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ASSESSMENT OF ORGANIC CONTAMINANTS IN EMISSIONS FROM REFUSE-DERIVED FUEL COMBUSTION

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16. ABSTRACT

Organic contaminants in emissions from refuse-derived fuel combustion were investigated in a 20-inch-diameter atmospheric fluidized-bed combustor. Combinations of coal/EcoFuel/MSW/toluene were burned in the combustor with temperatures ranging from 1250 to 1550°F. A Source Assessment Sampling System (SASS) was used to sample the stack gas; Level 1 methodology was used to analyze the organic contaminant levels. Combustion efficiencies of 93 to 98 percent were achieved in the test burns. Combustion of the EcoFuel generated fewer organic emissions than combustion of coal at similar combustion temperatures. The fine particulate collected by the SASS train filter contained higher concentrations of extractable organics than the reactor fly ash and the SASS cyclone samples. Combustion of a toluene/EcoFuel mix generated a large number of benzene derivatives not seen in the combustion of pure EcoFuel. Polycyclic aromatic hydrocarbons were the dominant organic compounds contained in the XAD-2 resin extract from coal combustion. A number of different priority pollutants were identified in the samples collected.

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FOREWORD

Today's rapidly developing and changing technologies and industrial products and practices frequently carry with them the increased generation of solid and hazardous wastes. These materials, if improperly dealt with, can threaten both public health and the environment. Abandoned waste sites and accidental releases ot toxic and hazardous substances to the environment also have important environmental and pubic health implications. The Hazardous Waste Engineering Research Laboratory assists in providing an authoritative and defensible engineering basis for assessing and solving these problems. Its products support the policies, programs and regulations of the Environmental Protection Agency, the permitting and other responsibilities of State and local governments and the needs of both large and small business in handling their wastes responsibly and economically.

Organic contaminants in emissions from refuse-derived fuel combustion were investigated in a 20-inch-diameter atmospheric fluidized-bed combustor. Combinations of coal/eco fuel/municipal solid waste/toluene were burned in the combustor with temperatures ranging from 1250° to 1550°F. A Source Assessment Sampling System was used to sample the stack gas; Level 1 Methodology was used to analyze the organic contaminant levels.

The information contained herein will be of interest to those designers or users who are contamplating or working with a system similar to this co-firing system. Requests for further information regarding the production and utilization of refuse-derived fuel should be directed to the Thermal Destruction Branch, HWERL, Cincinnati.

David G. Stephan, Director
Hazardous Waste Engineering Research Laboratory

ABSTRACT

Organic contaminants in emissions from refuse-derived fuel combustion were investigated in a 20-inch-diameter atmospheric fluidized-bed combustor. Combinations of coal/EcoFuel/MSW/toluene were burned in the combustor with temperatures ranging from 1250 to 1550° F. A Source Assessment Sampling System (SASS) was used to sample the stack gas; Level 1 methodology was used to analyze the organic contaminant levels. Combustion efficiencies of 93 to 98 percent were achieved in the test burns. Combustion of the EcoFuel generated fewer organic emissions than combustion of coal at similar combustion temperatures. The fine particulate collected by the SASS train filter contained higher concentrations of extractable organics than the reactor fly ash and the SASS cyclone samples. Combustion of a toluene/EcoFuel mix generated a large number of benzene derivatives not seen in the combustion of pure EcoFuel. Polycyclic aromatic hydrocarbons were the dominant organic compounds contained in the XAD-2 resin extract from coal combustion. A number of different priority pollutants were identified in the samples collected.

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I. PROGRAM OBJECTIVES

The primary objectives of this study were to assess organic and trace metal emissions from the combustion of refused-derived fuels (RDF) in an atmospheric fluidized-bed combustor (AFBC). A total of four fuels were used in the test program, namely coal, EcoFuel, MSW, and reagent grade toluene. A Source Assessment Sampling System (SASS) was used to collect the samples (solid and liquid) for organic and trace metal analysis.

Because of funding limitations for the program, the SASS samples were analyzed for organic content only and no trace metal analyses were performed. A Level 1 approach was used to characterize the organic content of the RDF combustion effluents; the Level 1 methodology is described in detail in Section IV of this report.

II. DESCRIPTION OF EQUIPMENT

A. ERCO Fluidized-Bed Pilot Plant Facility

A schematic of the ERCO 20-inch diameter AFBC is shown in Figure 1. The solid fuel is shredded to the desired size in the William's hammermill. The sized feedstock is then loaded into a feed hopper. The material is then fed through a rotary valve into an Acrison metering screw which directly discharges into the lower section of the fluidized bed. In the run in which liquid toluene was added to the reactor, a tank was pressurized with N_2 and the liquid toluene was metered through a rotameter and then injected directly into the bed through a small orifice. Combustion air is provided by a positive displacement blower and is metered by an Erdco

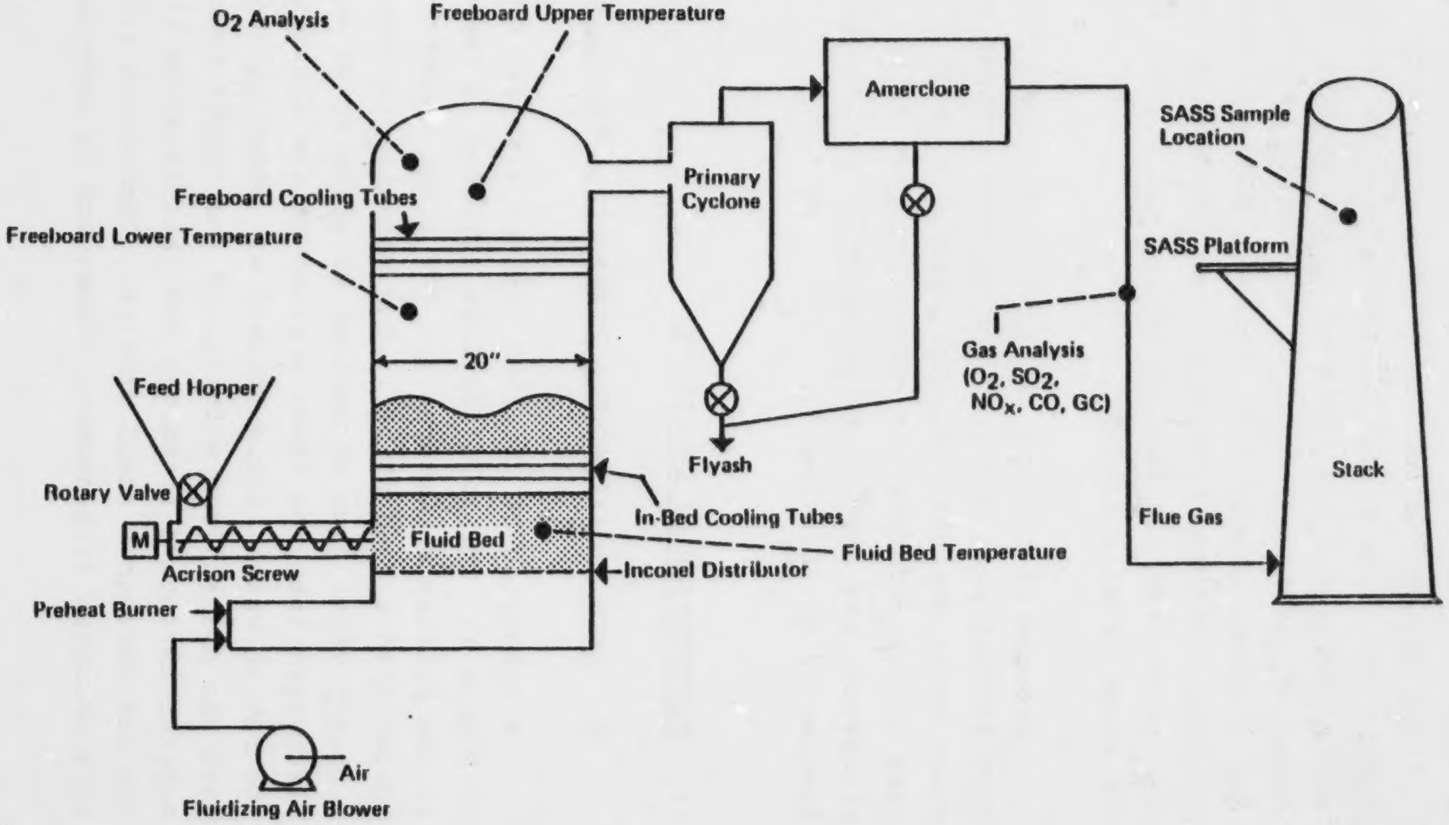
O_2 Analysis
Freeboard Upper Temperature
Freeboard Cooling Tubes
Freeboard Lower Temperature
20"
Feed Hopper
Rotary Valve
M
Acrison Screw
Fluid Bed
Preheat Burner
Air
Fluidizing Air Blower
Primary Cyclone
Amerclone
Flyash
In-Bed Cooling Tubes
Fluid Bed Temperature
Inconel Distributor
Gas Analysis (O_2, SO_2, NO_x, CO, GC)
Flue Gas
SASS Sample Location
SASS Platform
Stack

Figure 1. Pilot Plant Schematic.

flowmeter which was previously calibrated with SO_2. A start-up burner is used to preheat the bed sand to 800-900° F before the introduction of the solid fuel.

The fluidized-bed reactor is a refractory-lined vessel 20 inches in inside diameter and approximately 20 feet high. A perforated Inconel plate is used as the combustion air distributor. Refractory grog, a high Al_2O_3 material, is employed as the bed material.

The average particle size of the bed sand is approximately 420 microns. A static bed height of 17 to 22 inches was employed for the runs; this corresponds to a fluidized-bed height of 26 to 36 inches at a typical fluidizing velocity of 2.7 to 4.4 feet per second. Pressure taps were employed to quantify the mass of sand/fuel present in the bed during the course of a run. Water-cooled tubes (1.5 inch diameter) were installed in-bed (two separate circuits) and in the freeboard (ten tubes on a single circuit) in order to maintain the bed at the desired temperature and to limit the cyclone inlet temperature, respectively. Rotameters and thermocouples were employed to quantify the heat removal by the various tube circuits. A number of thermocouples were installed in the bed section to characterize the quality of fluidization; thermocouples were also installed below and above the freeboard tubes in order to indicate the extent of freeboard burning.

The hot-particulate-laden off-gasses (850 to 1300° F) were then sent to a primary cyclone (Fisher Klosterman Type XQ-465) and then to secondary Amerclones. Fly ash captured by the cyclones was collected in drums which were weighed at the completion of the run to determine the rate of fly ash discharge. The cyclone discharge gases were then sent to the stack. No induced-draft fan or baghouse was used in these runs.

B. ERCO Pilot Plant - Analytical Support

A number of analytical devices were used to monitor and quantify the combustion runs. The equipment used to measure the off-gas composition (O_2, SO_2, NO_x, CO) and the sampling locations are summarized in Table 1. The techniques employed for characterizing the solid sample (feedstock and fly ash) are also summarized in Table 1.

C. SASS Train

An Acurex SASS train was used to collect the particulate and organic emissions from the stack gas. The SASS train is described in detail by Blake (1977); a brief description will be provided in this section. A schematic of the SASS train is shown in Figure 2. The major components include (1) a stainless steel heated probe, (2) three cyclones in series (10 mm, 3 mm, 1 mm cut diameters) and a filter enclosed in a thermostatically controlled oven (400-450° F), (3) the organic module, which consists of a gas cooler (for the Level 1 procedure the gas is cooled to 68° F), a sorbent cartridge for adsorbing the organic compounds (typically 100 g of 80 mesh XAD-2 ion exchange resin), and a condensate trap which collects liquid condensed from the cooled gas sample. The gas is cooled to 68° F before contacting the resin by circulating ice water from the impinger bath. The cooled gas is then sent to four impingers in series, which are used to collect samples for trace metal analysis and drying the gas before it enters the vacuum pumps and the gas meter. The impingers are contained in an ice bath. The contents of the first three impingers are as follow:

Impinger #	Contents
1	Hydrogen Peroxide
2 & 3	Ammonium Persulfate/ Silver Nitrate

TABLE 1

ERCO PILOT PLANT ANALYTICAL EQUIPMENT

COMPONENT	EQUIPMENT	SAMPLING LOCATION	MODE
GAS COMPOSITION			
O_2	Teledyne, Beckman	Freeboard/ Stack	Continuous
SO_2	Thermal Electron Pulsed Fluorescent	Stack	Continuous
CO	Thermal Electron Infrared	Stack	Continuous
NO_x	Teledyne Chemilumescent	Stack	Continuous
CH_4, C_2, C_3, O_2, N_2, CO	Fisher Gas Partitioner	Stack	Batch

SOLID SAMPLES

Heating Value - Paar Bomb Calorimeter
Proximate Analysis (Volatiles, Ash) - ASTM standards
Ultimate Analysis (CHNOS) - atomic adsorption
Moisture - moisture balance

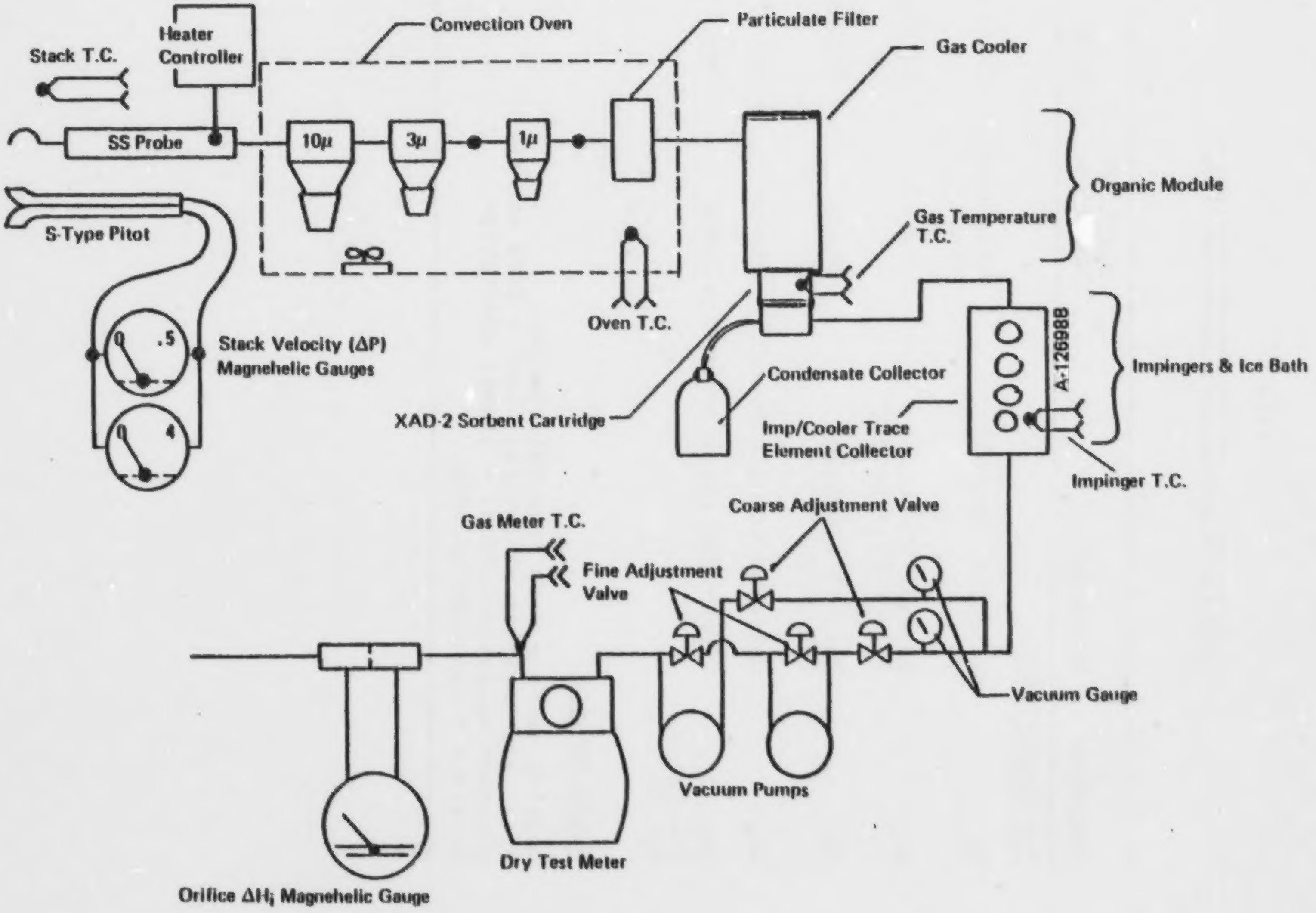
Stack T.C.
Heater Controller
Convection Oven
Particulate Filter
Gas Cooler
SS Probe
10μ
3μ
1μ
Organic Module
S-Type Pitot
Gas Temperature T.C.
Oven T.C.
0
.5
0
4
Stack Velocity (ΔP) Magnehelic Gauges
A-126988
Impingers & Ice Bath
Condensate Collector
XAD-2 Sorbent Cartridge
Imp/Cooler Trace Element Collector
Impinger T.C.
Coarse Adjustment Valve
Gas Meter T.C.
Fine Adjustment Valve
Vacuum Gauge
Vacuum Pumps
Dry Test Meter
Orifice ΔHi Magnehelic Gauge

Figure 2. SASS Flow Diagram.

There are the recommended solutions for the Level 1 Environmental Assessment. The fourth impinger was filled with 3-8 mesh indicating silica gel.

The dry gas from the final impinger was then pumped with two vacuum pumps in parallel through a dry test meter and then passed through an orifice plate which was used to instantaneously record/adjust the flowrate through the SASS system.

The entire SASS system was leak checked (less than 0.05 to 0.10 CFM leak rate at 15 inches Hg) and the system tightened up before initiating a SASS run.

The recommended sampling rate for the SASS system is 4 SCFM; there was no problem with obtaining this rate when the filter was clean but, because of the particulate loading in the stack, it was necessary to change the filter a number of times during the course of the run (3 to 5 times) in order to maintain the desired rate. Because of this filter blockage problem, two decisions were made. The first was that the filter would be changed when the sample rate was reduced to 2.8 SCFM (with the pumps wide open); this resulted in an average sampling rate of 3.1 to 3.9 SCFM over the course of a run. The total sampling time was generally 240 minutes (except for one run which was only 148 minutes due to operational problems).

The other major problem with the original Acurex SASS train was that the filter was located in the oven with the three cyclones such that every time it was changed, (1) it required an inordinate changeover time (60-90 minutes) and (2) the technician usually burned his arms in trying to maneuver an adjustable wrench in the very close quarters.

This procedure was incredibly painful. This problem was remedied by installing the filter in a separate oven situated on top of the existing SASS oven. This enabled a 30-minute changeover time and eliminated personnel injury. The line from the third cyclone to the filter was heat traced to avoid condensation of organic vapors.

D. ERCO Environmental Laboratory Organic Analysis Equipment

The samples which were collected from each combustion run included the following:

Source	Identification	Type
Feedstock	Feedstock	Solid
SASS	XAD-2 Resin	Solid
SASS	Combined Cyclones	Solid
SASS	Particulate Filter	Solid
SASS	Organic Trap Condensate	Liquid
Reactor Cyclone Catch	Fly Ash	Solid

The three SASS cyclone samples were combined to reduce the analytical cost. The impinger samples were collected and saved but because of funding limitations, they were not analyzed for trace metal. The ERCO laboratory equipment for the Level 1 organic analysis included (1) a Hewlett-Packard 5840 GC equipped with a flame ionization detector, (2) a Perkin Elmer 283 double beam infrared spectrophotometer and (3) a Hewlett-Packard 5985 quadropole GC/MS/DS. The organic analyses were performed in-house by the ERCO Environmental Laboratory. The Level 1 procedure is described in more detail in Section IV of this report.

III. DESCRIPTION OF FEEDSTOCKS FOR COMBUSTION TESTING

The three solid feedstocks employed in the AFBC testing were Battelle Coal, EcoFuel provided by Combustion Equipment Associates, and MSW provided by Americology. Reagent grade toluene was also used to simulate combustion of a hazardous waste. The properties of the solid fuels (size, HHV, moisture, ultimate analysis, and fusion temperature) are summarized in Table 2.

The test runs were performed with feedstock mixes shown in Table 3.

The feedstock mixes (except for run 25) were prepared by mixing the respective fuels on the floor with a shovel and/or bobcat. As noted previously, the toluene was injected into the fluidized bed through a small orifice from a tank pressurized with N_2; the toluene flowrate was monitored with a rotameter.

It is noted that the Americology MSW has a fusion point around 1300° F due to the glass content of the material. In a previous ERCO program with the same MSW, it was found that fluidization problems were incurred if the bed temperature exceeded nominally 1300° F; for this reason, the combustion runs with MSW were performed at a temperature slightly less than this fusion temperature.

TABLE 2

COAL/RDF SUPPLIERS AND FUEL PROPERTIES

	FEEDSTOCK		
	CRUSHED COAL	ECOFUEL	AMERICOLOGY
Supplier	Battelle	Combustion Equipment Associates	American Can
Size	23%>1.7 μm 59% mid-range 18%>300 μm	27%<170 mesh 30% 170/230 mesh 42% 230/325 mesh	<1"
Heating Value (HHV, Btu/lb m.f.)	12953	7827	6430
Moisture (% wet basis)	8.11	4.7	26.6
Ultimate Analysis (wt %, m.f.)			
Sulfur	1.4	0.61	0.3
Carbon	74.2	40.0	51.0
Hydrogen	4.9	4.6	6.8
Nitrogen	1.3	<0.1	0.7
Oxygen	9.0	45.5	26.0
Chloride	--	0.26	--
Ash	9.2	9.0	15.2
Fusion Temperature (°F)	--	~1800	~1300

TABLE 3

FEEDSTOCK MIX COMPOSITION

RUN ID	COAL	ECOFUEL	MSW	TOLUENE	TOTAL
17	50	50	--	--	100
18	100	--	--	--	100
22	100	--	--	--	100
23	50	--	50	--	100
24	--	100	--	--	100
25	--	82	--	18	100

IV. EXPERIMENTAL PROCEDURES

A. Pilot Plant Combustion Tests

After the feedstock was shredded, the fluidized bed was preheated to 800-900° F with hot combustion gases from the preheat burner located below the Inconel distributor plate. The feedstock mix was then added to the hopper above the rotary star valve; for the runs which used MSW, the static head was minimized to prevent bridging of the material in the hopper. The flowrate of the combustion/fluidizing air was metered by an Erdco flowmeter. The flowrate of the solid fuel was determined by (1) calibration of the Acrison metering screw, (2) averaging the total weight of material fed over the duration of the run, and (3) monitoring the rate of feed addition (with preweighed 5-gallon buckets) to the hopper. With this procedure, it was possible to quantify the feedrate within ±10 percent. Typical solid feedrates to the AFBC ranged from 40 to 70 lb/hr. As noted in Section VIII, it is advisable to employ a weigh belt and to utilize pneumatic injection to more accurately quantify the solid feedrate.

The average fluidizing velocity (at bed conditions) ranged from 2.7 to 4.4 fps. The excess air (based on the excess O_2 in the stack gases) ranged from 35 to 60 percent.

The bed temperature was maintained at 1500-1550° F for the runs with coal, EcoFuel, and toluene (except for run 22 with coal at 1250° F); the bed temperature for the MSW run was maintained at 1250° F (below the glass fusion point).

Typically, the AFBC was operated for 3-4 hours in order to establish reasonable steady-state conditions (primarily reactor heat-up) before the initiation of the run and SASS sampling. Since the total SASS sampling time was 4 hours, and a number (3 to 5) of SASS filter changes were made, each one requiring 30-45 minutes, this meant that the elapsed time for the SASS sampling was 6-8 hours. Thus the total time for each run was 9-12 hours.

During the SASS sampling, the oven temperatures (cyclone and filter ovens) were monitored and controlled at 400-450° F. The organic module was maintained at 68° F ± 2° F by ensuring there was sufficient ice in the impinger bath. The organic module condensate trap was drained periodically to prevent overflow of liquid from the trap to the impingers. The initial SASS sampling rate was set at 4.0 SCFM. Usually after 30-60 minutes, the flow was reduced to 2.7 SCFM (arbitrary cut-off point) even with the vacuum pumps wide open. At this time, the filter was changed and, after reheating the filter oven (10-15 minutes) to 400-450° F, the run was continued.

It was not necessary to drain bed material from the reactor during the progress of the run since the input ash was elutriated at a sufficient rate.

Because of the desire to accurately quantify the solid fuel feed rate, it was decided to perform a trial run(s) at the desired run conditions before performing the SASS run. This trial run(s) was carried out in order to (1) assess and remedy feed problems (particularly the MSW), (2) establish the proper metering screw setting at actual run conditions, and (3) ascertain whether a lower fluidization velocity was required because of excessive freeboard burning (a phenomenon associated with the fine EcoFuel) due to excessive elutriation of the feedstock.

During the actual test run, the gas composition (O_2, NO_x, CO, SO_2) was continuously monitored (refer to Table 1) and grab samples were taken for GC analysis (CH_4, C_2, C_3).

The SASS samples (cyclone, particulate filter, organic module condensate, XAD-2 resin, and impinger solutions) were generally allowed to still overnight with the system sealed. The next day, the SASS samples were weighed and stored in their respective containers for subsequent organic analysis. Before putting the samples in their containers, the containers were "cleansed" of organic contamination by following the recommended Level 1 procedure. Typically, it took one and a half days for the SASS samples to be weighed, stored, and the SASS system cleaned out. Another half-day was required to reassemble the SASS train, leak-check, and install the train on the stack platform located about 20 feet from ground elevation.

B. Organic Analysis - Level 1 Procedure

Analysis of the SASS samples and the reactor fly ash sample was performed by the Level 1 methodology developed by EPA-IERL (1978). The samples which were analyzed included the (1) XAD-2 resin, (2) combined cyclones, (3) particulate filter, (4) organic trap condensate, (5) reactor fly ash and (6) the feedstocks. A summary of these methods is shown in Figure 3.

Solid samples and the XAD-2 resin were extracted for 24 hours in a Soxhlet apparatus using methylene chloride. Aqueous solutions (organic trap condensates) were extracted in separatory funnels using methylene chloride after adjusting the aqueous pH first to 2 and then to 11. Procedural blanks

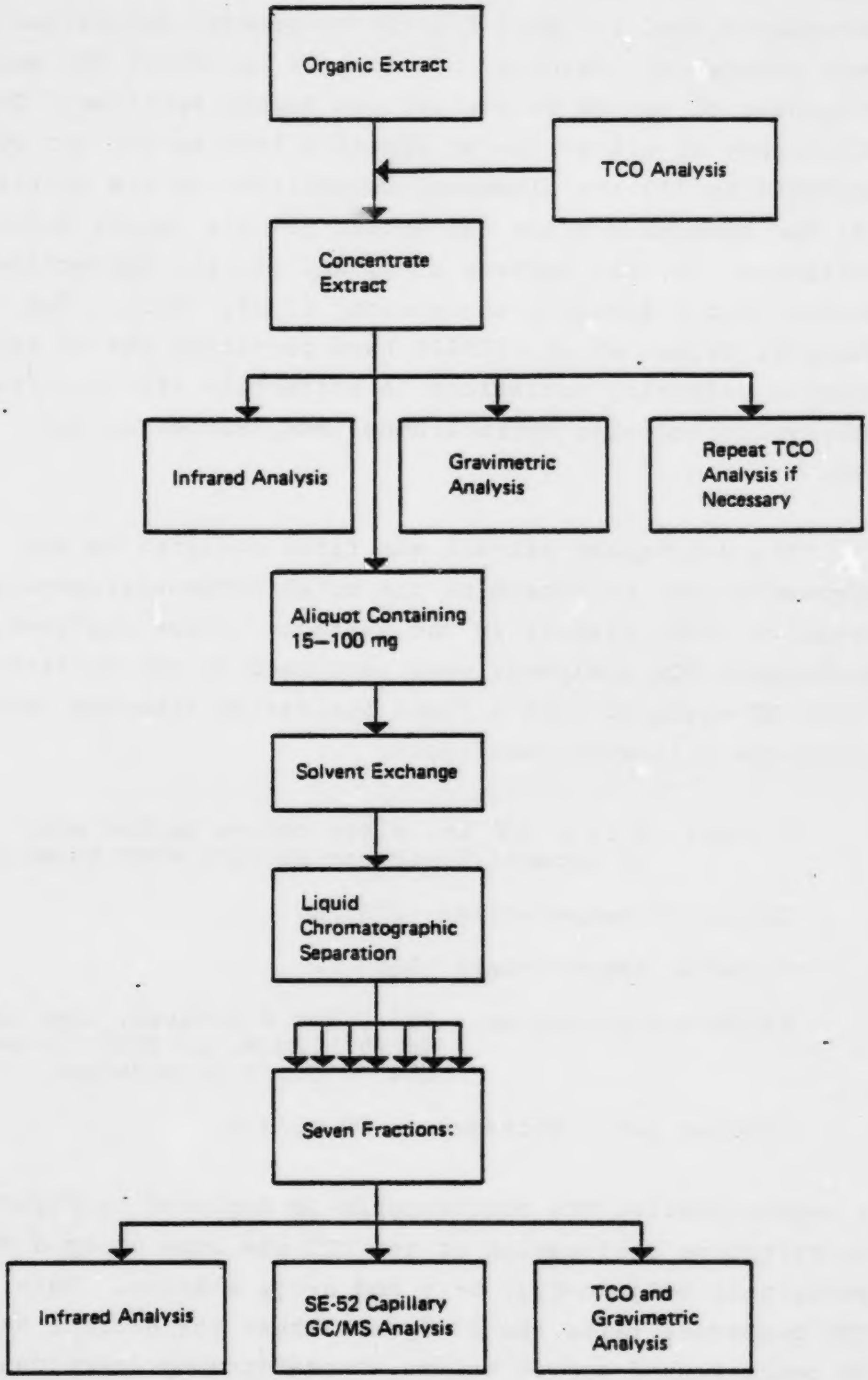
Organic Extract
TCO Analysis
Concentrate Extract
Infrared Analysis
Gravimetric Analysis
Repeat TCO Analysis if Necessary
Aliquot Containing 15—100 mg
Solvent Exchange
Liquid Chromatographic Separation
Seven Fractions:
Infrared Analysis
SE-52 Capillary GC/MS Analysis
TCO and Gravimetric Analysis

Figure 3. Level 1 Organic Analysis Methodology (EPA, 1978).

were prepared with the samples to insure no contamination was occurring. It should be noted that the extraction procedures used in Level 1 focus on general recoveries of most classes of organics, but are not optimized for each component contained in the various sample matrices. The efficiency of extraction of organics from solids can be affected by (1) the elemental composition of the particles, (2) the compounds being extracted, (3) the amount being extracted, (4) the solvent used, and (5) the extraction method (e.g., Soxhlet, sonication) (Junk, 1981). For example, Griest et al. (1980) have performed one of many studies examining variations in extraction efficiencies for polycyclic aromatic hydrocarbons (PAH) sorbed on fly ash.

The subsequent extract was first analyzed by gas chromatography to determine the total chromatographable organics (TCO) present in the extract. These analyses, and subsequent TCO analyses, were performed on our Hewlett-Packard 5840A GC equipped with a flame ionization detector (FID) using the following conditions:

Column: 6 ft x 1/8 in. glass column packed with 10 percent OV-101 on 100/120 mesh Supelcoport.

Injection temperature: 275° C.

Detector temperature: 300° C.

Temperature program: 30° C for 6 minutes, then programmed at 20° C/min. to 250° C, and held at 250° C for 5-10 minutes.

Carrier gas: Nitrogen at 30 ml/min.

A representative TCO chromatogram is depicted in Figure 4. Quantitative calibration of the TCO was done using a standard containing n-C_8, n-C_{12}, n-$_{17}$ and n-C_{18} alkanes. This initial TCO procedure tells the analyst whether the extract needs to be concentrated before column chromatography fractionation (any quantities greater than 2 milligrams are not concentrated),

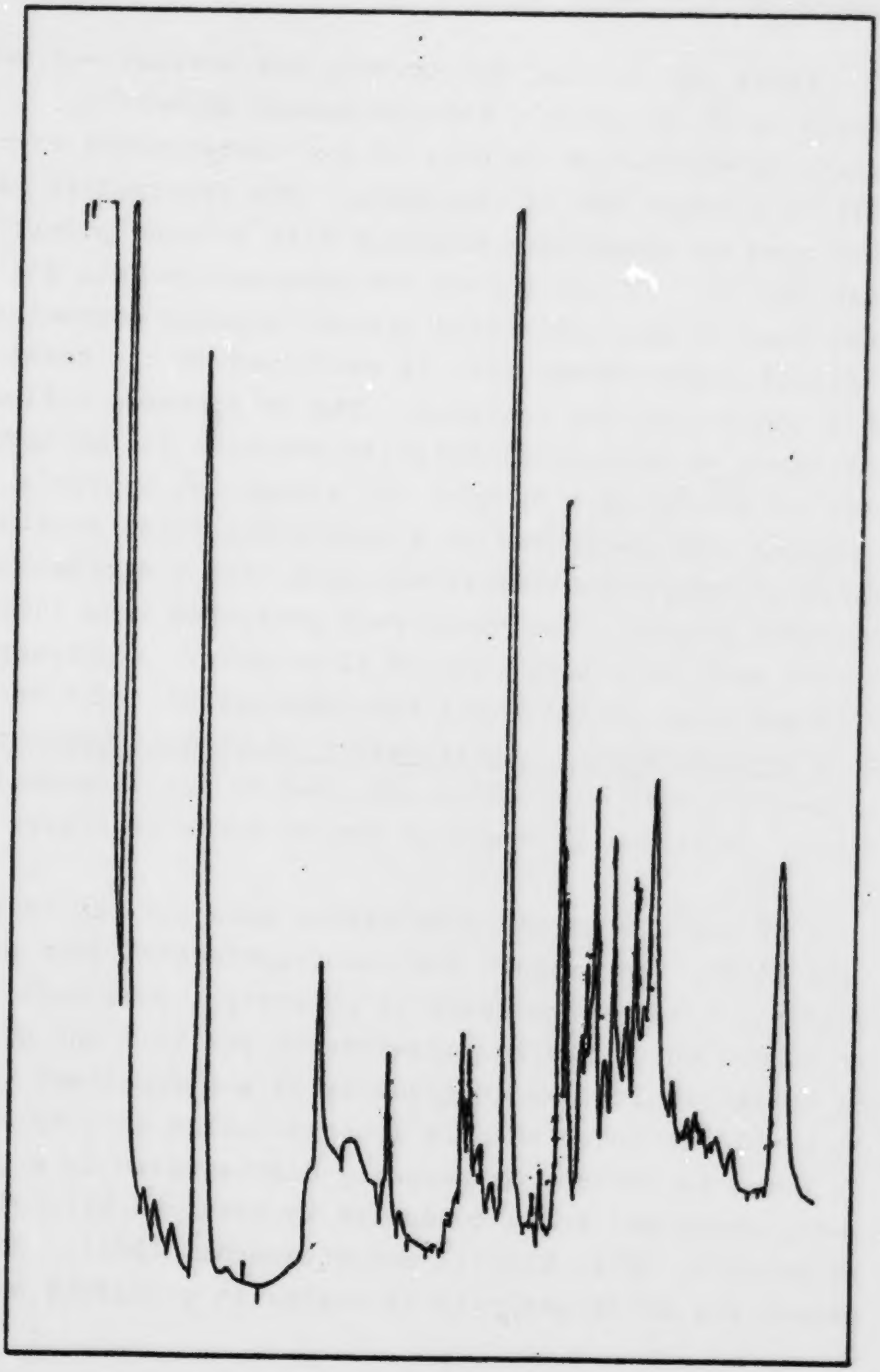

Figure 4. TCO Chromatogram of Sample 27-009, f_3 (Combined Cyclone).

and will eventually be used to quantitate organics with boiling points ranging from 100° to 300° C.

After the initial TCO screen, the extract was concentrated to 10 ml using a Kuderna-Danish apparatus. A gravimetric determination is done on the concentrated extract, as well as another TCO if necessary. The gravimetric data is then used to quantitate organics with boiling points higher than 300° C. If the sum of the gravimetric data and TCO is less than 15 mg, indicating minimal organic contamination, then infrared spectroscopy (IR) is performed on the total extract, thus completing the analysis. The IR spectrum indicates the types of functional moieties presents in the sample, as well as providing a control for subsequent analysis. The IR analyses were performed on a Perkin-Elmer 283 double-beam infrared spectrophotometer equipped with a microprocessor and NaCl plates. The scans were performed from 4000 cm^{-1} to 200 cm^{-1} at a scan rate of 12 minutes. A polystyrene film was used to calibrate the instruments. The reference book Spectrometric Identification of Organic Compounds (Silverstein et al., 1974) was used to aid in peak identifications. A sample IR spectrum can be found in Figure 5.

If the sum of the gravimetric data and TCO is greater than 15 mg, the extract must be fractionated into similar chemical classes according to polarity. Then each fraction is subjected to TCO and gravimetric analysis and depending on those results, is analyzed by IR and capillary GC/MS. It should be noted that IR interpretation of complex samples is prone to errors, as recently demonstrated in a Level 1 interlaboratory study conducted by Research Triangle Park (Gutknecht, 1979; Gaskill and Gutknecht, 1981). For this reason the GC/MS analysis is useful in providing corroborative

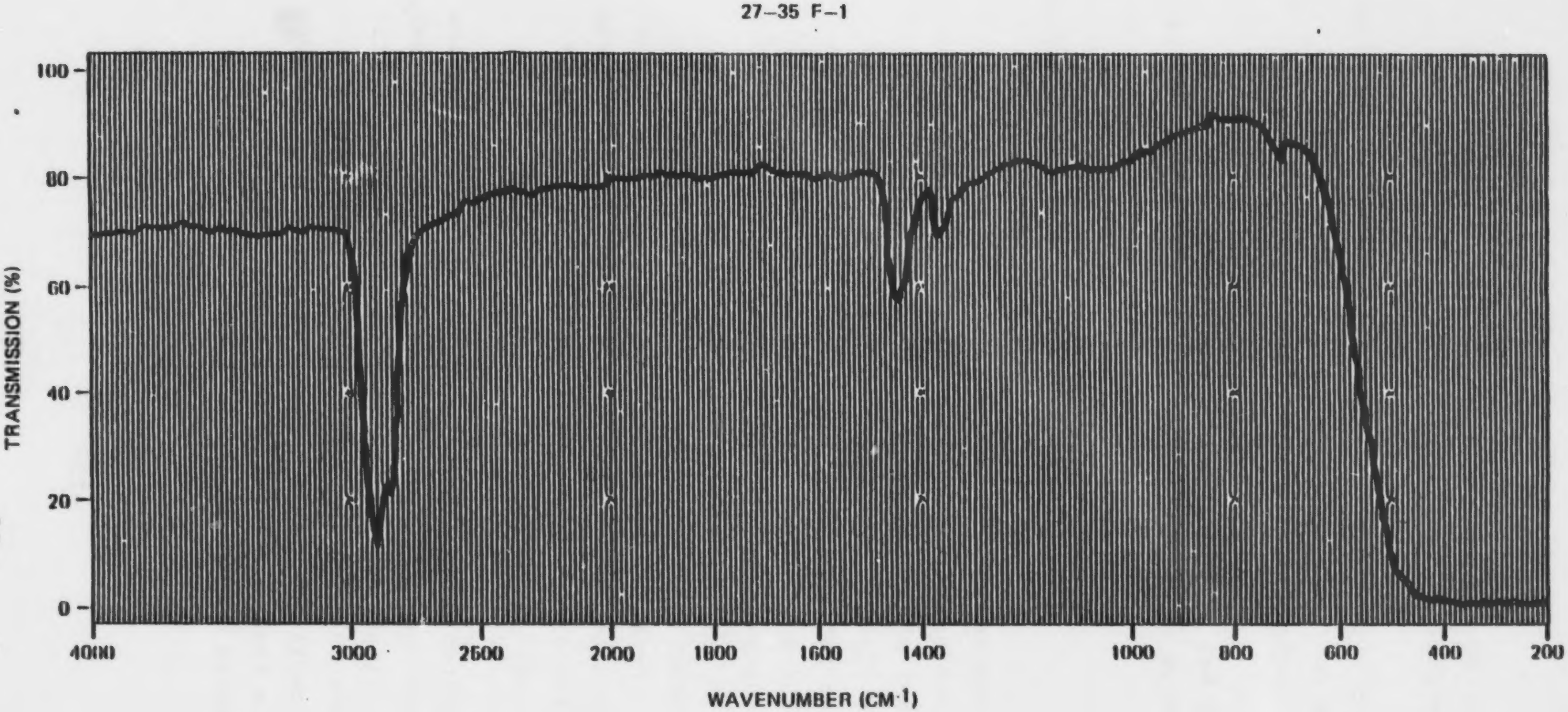

Figure 5. IR Spectra of Sample 27-035, f-1.

information for IR, as well as supplemental data for additional identifications.

To proceed with the column chromatography procedure, an aliquot of the concentrated methylene chloride extract is first solvent exchanged to cyclopentane. The extract is then placed onto a glass column containing 6 grams of Davison Silica Gel (60/200 mesh, Grade 950) topped with 3 grams of sodium sulfate, and then eluted in the following order:

Fraction	Solvent(s)	Volume (ml)
f_1	Pentane	25
f_2	20% methylene chloride in pentane	10
f_3	50% methylene chloride in pentane	10
f_4	Methylene chloride	10
f_5	5% methanol in methylene chloride	10
f_6	20% methanol in methylene chloride	10
f_7	50% methanol in methylene chloride	10

A solution containing 1-hexadecanol, ethylene glycol, naphthalene, linoleic acid, dodecane, acetonitrile, tetrahydrofuran, dioxane, benzaldehyde and n-butyl phthalate was used intermittently to insure the fractionation procedure was being employed properly.

The suggested Level 1 mass spectral analysis is by low resolution mass spectrometry using a direct probe. However, the recent developments in the field of fused-silica capillary GC columns makes this type of analysis attractive. Fused-silica capillary columns are superior to pack columns by providing a higher degree of peak resolution and increased inertness (Jennings, 1980; Lipsky et al., 1980).

Because capillary GC columns have been successfully used for complex environmental samples (e.g., Yu and Hites, 1981), it was felt that more useful information could be derived from this techique rather than the direct probe low resolution method suggested by EPA. The analyses were performed on a Hewlett-Packard 5985 quadropole GC/MS/DS using the following conditions:

Column: 30 m SE-52 fused silica column, .25 mm I.D.
(J&W Scientific Co.)

Injection temperature: 250° C

Transfer line temperature: 300° C

Temperature program: 40 to 290° C at 10°/min

Carrier gas: Helium at 2 ml/min.

Ionization voltage: 70 eV

Electron multiplier voltage: 2200 V

Scan conditions: 40 amu to 500 amu at 225 amu/sec

Tuning standard: PFTBA

Internal standard: d_{10} anthracene

Attempts were made to identify the 10-15 largest peaks in each GC/MS analysis. Identifications were made from the fragmentation patterns using the Registry of Mass Spectral Data (Stenhagen, 1974) and the Eight Peak Index of Mass Spectra (Mass Spectrometry Data Centre, 1974). Quantitative analysis was complicated by the complex matrix encountered in combustion products. It would be quite difficult to anticipate and procure standards needed for all compounds that may be encountered, as well as ascertain extraction efficiencies. However, estimated concentrations were produced using response factors of similar compounds which are analyzed routinely, in this case d_{10}-anthracene. A sample GC/MS chromatogram is illustrated in Figure 6.

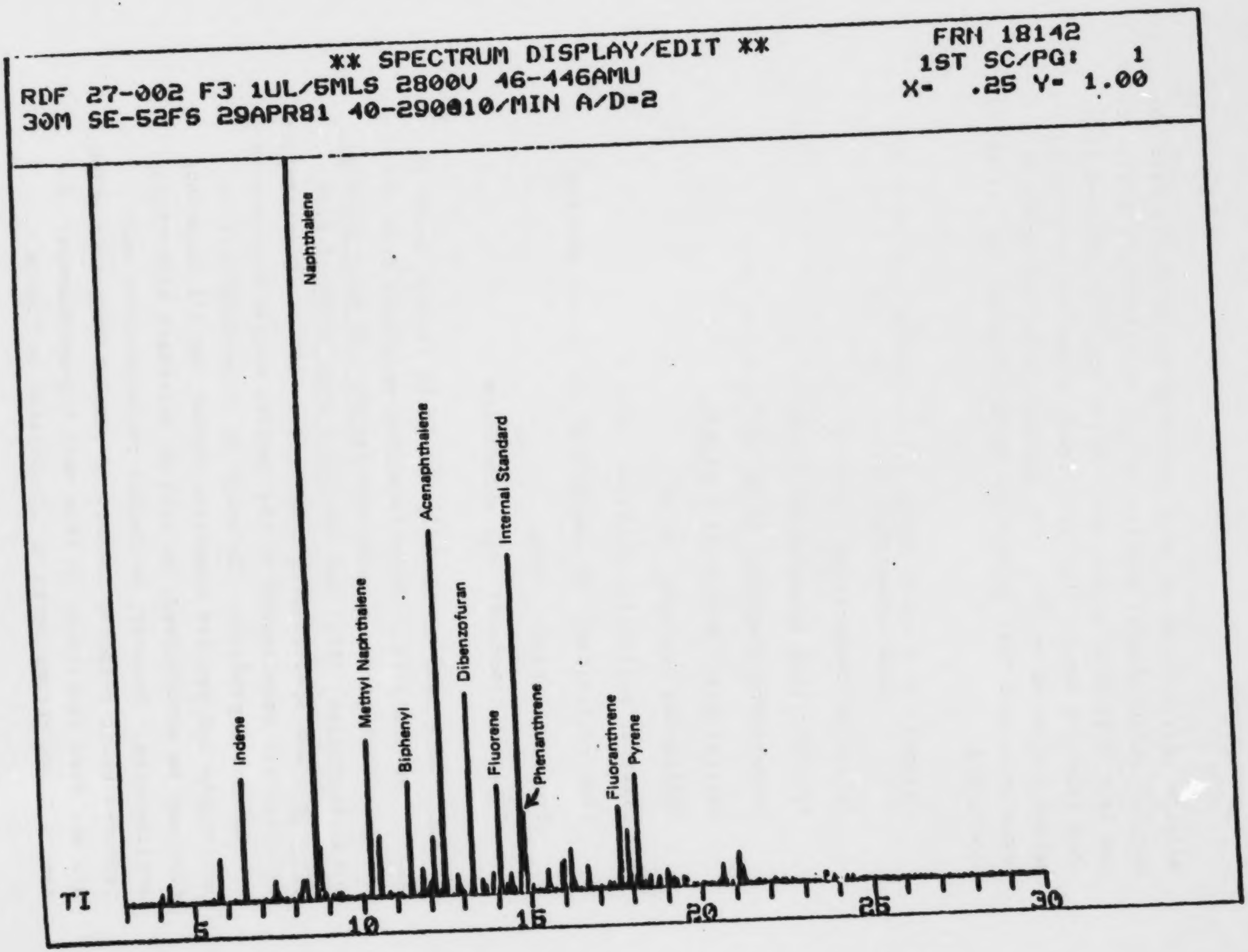

Figure 6. GC/MS Chromatogram of Sample 27–002, f_3 (XAD-2 Resin).

V. EXPERIMENTAL RESULTS

A. Pilot Plant Combustion Tests

The six runs for which the complete SASS analysis was performed are summarized in Table 4 for the various coal/ EcoFuel/MSW/toluene mixtures. This table summarizes the air and fuel feedrates, reactor temperatures, fluidization conditions, off-gas composition, fly ash collection, emission rates for SO_2 and NO_2 (lb/MMBtu), and the overall carbon burn-up efficiency. A computer program was developed to do the heat and material balance for each of the runs, and Table 4 is a summary of the computer output from each of the runs. The results of this table are discussed in Section VI.

A summary of the SASS data is provided in Table 5 for each of the six runs. The particulate weights are quite accurate whereas the relative amounts of liquid in the impingers, silica gel, and organic module condensate are tenuous since the impingers were sometimes inadvertently back-flushed during the SASS sampling. Table 5 also summarizes the normalized rates [grams of material collected from the SASS (either liquid or solid) per pound of fuel (combined mixture if more than one feedstock (as received basis))]. These quantities were determined from the SASS data as follows:

Normalized Rate defined as:

$$\frac{\text{grams material}}{\text{pound fuel}} = \frac{\text{grams material}}{\text{DSCF sampled}} \times \frac{\text{DSCF}}{\text{pound fuel}}$$

The first term in parentheses on the righthand side was determined from the SASS data in Table 5; the second term in parentheses was determined from the data in Table 4. These normalized rate values are used in conjunction with the organic analyses to calculate the organic emission rates for the various runs (refer to Section V B).

TABLE 4

SUMMARY OF ERCO PILOT PLANT COMBUSTION DATA

Run ID	17	18	22	23	24	25
Date	5/23	5/28	6/24	6/27	7/22	8/7
Feedstock Composition (wt %)						
Coal	50	100	100	50	—	--
EcoFuel	50	—	—	—	100	82
MSW	—	—	—	50	—	—
Toluene	—	—	—	—	—	18
Total	100	100	100	100	100	100
Total Fuel Feedrate (pph)	69	56	36	53	59	62
Combustion Air Flow (SCFM)	144	144	104	104	87	104
Temperatures (°F)						
Bed	1500	1500	1250	1250	1500	1550
Freeboard Lower	1550-1570	1520-1535	1350	1330-1360	1530-1650	1560-1570
Freeboard Upper	1320	1181	854	888	960	990
Fluidization Conditions						
Velocity (fps)	4.4	4.3	2.7	2.7	2.8	3.3
Static Bed Height (inches)	17	17	18	17	20	22
Bed ΔP ("WC)	21	21	23	22	26	28
Distributor ΔP ("WC)	32	34	49	50	32	37
Off-Gas Composition						
SO_2 (ppm)	750	684	529	455	558	400
NO_x (ppm)	216	290	277	278	117	125
CO (ppm)	1466	2043	559	1506	507	720
O_2 Percent (% XS Air)	5.4 (35)	6.8 (48)	7.8 (59)	6.0 (40)	7.0 (50)	6.5 (45)
Flyash Collected						
Rate (pph)	6.8	8.5	4.8	7.5	5.8	5.0
Volatiles (wt %)	3.3	8.1	6.8	3.8	4.3	--
Ash (wt %)	87.6	56.8	65.0	74.8	90.0	90.0
Grams Fly Ash/lb Fuel	44.7	68.9	60.5	64.2	44.6	36.6
Emissions (lb/MMBtu)						
SO_2	1.72	1.51	1.29	0.98	1.23	0.77
NO_2	0.36	0.46	0.49	0.43	0.18	0.17
Carbon Burn-Up (%)[a]	97	90	93	93	97	98
Overall Heat Balance (Q_{out}/Q_{in})[b]	0.93	0.80	0.58	0.64	0.50	0.82

[a] Defined as (carbon out in gas/carbon introduced with feed) x 100.

[b] Defined as total heat out (flue gases, fly ash, cooling water)/HHV of feedstock in.

TABLE 5

SUMMARY OF SASS DATA

Run ID	17	18	22	23	24	25
Run Date	5/23	5/28	6/24	6/26	7/22	8/7
Coal/Eco/MSW/Toluene	50/50/0/0	100/0/0/0	100/0/0/0	50/0/50/0	0/100/0/0	0/82/0/18
Sampling Time (min.)	240	148	237	253	237	238
DSCF Sampled	839	462	750	818	932	824
DSCFM (average)	3.5	3.1	3.2	3.2	3.9	3.5
Particulate (grams)						
10- m Cyclone	23.599	6.93	10.36	9.619	9.25	8.6
3- m Cyclone		16.444	19.565	24.186	21.2	15.6
1- m Cyclone	16.003	16.845	28.451	25.271	15.03	6.55
Filter[a]	5.189(4)	4.766(5)	4.468(5)	3.054(4)	0.92(3)	1.45(3)
Total (grams)	44.79	44.985	62.84	62.13	46.40	32.2
Liquid Collected (grams)						
Impingers	+40	+25	-20	+540	+115	+210
Silica Gel	+132	+159	+8.4	+4.9	+368	+310
OM Condensate[c]	1200	+300	N.A.	+560	+1240	+690
Total (grams)	+1372	+484	N.A.	+1105	+1723	+1210
XAD-2 Resin (grams)	105[d]	106	100	100	102	101
Normalized Rates[b]						
Combined Cyclones	5.900	13.4	13.5	8.51	4.29	3.75
Particulate Filter	0.773	1.59	1.03	0.440	0.087	0.177
OM Condensate	178	99	N.A.	81	117	84
XAD-2 Resin	N15.6	35.3	23.1	14.4	9.63	12.3

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[a] Number in parentheses is the number of filter changes

[b] The specific rates are grams of material/pound of feedstock (as is).

[c] OM X Organic Module Condensate.

[d] Assumed value.

B. Organic Analyses - Level 1 Procedure Results

A total of 33 samples were analyzed; these samples are summarized in Table 6. The preliminary analyses of the total extractable organic content (TEO) for the individual samples is summarized in Table 7. The organic content of the LC fractions for those samples whose sum of gravimetric data and TCO is greater than 15 mg is summarized in Table 8.

The IR screen for the original extracts of all samples is summarized in Appendix I; the IR screen for the fractionated extracts presented in Table 8 are summarized in Appendix II; the GC/MS data for fractionated extracts which were deemed to have significant organic content are summarized in Table 9. In addition GC/MS data are presented for some total extracts which were considered to have marginal organic content.

C. Organic Emission Rates

Using the normalized rates (grams/lb fuel) for the SASS samples (combined cyclone, particulate filter, OM condensate, and XAD-2 resin) in Table 5 and the reactor fly ash samples in Table 4 in conjunction with the total extractable organic content (TEO) in Table 7 (final column in Table 7), it is possible to calculate the organic emissions rates/pound feedstock (as is) for the pilot plant runs. The procedure for each sample is as follows:

$$\frac{\text{mg organic emitted}}{\text{lb fuel feed}} = \frac{\text{mg organic}}{\text{g sample}} \times \frac{\text{g sample}}{\text{lb fuel}}$$

The first term on the righthand side is from Table 7 and the second term on the righthand side is from either Table 4 or 5. A summary of these calculations is provided in Table 10 for each pilot plant run. The feedstock (averaged if a mixture) TEO is also provided. Also listed in Table 10 are the percentages of organics collected by the different SASS samples.

TABLE 6

SAMPLES ANALYZED FOR ORGANIC CONTENT

RUN ID	FLUIDIZED-BED FEEDSTOCK	ERCO LAB ID	SAMPLE
18	Pure Coal at 1500° F (May 28, 1980)	27-002	XAD-2 resin
		27-008	Combined cyclones
		27-014	Particulate filter
		27-020	Organic trap condensate
		27-026	Fly ash
		27-036	Coal feedstock
22	Pure Coal at 1250° F (June 24, 1980)	27-003	XAD-2 resin
		27-009	Combined cyclones
		27-015	Particulate filter
		27-021	Organic trap condensate
		27-027	Fly ash
		27-036	Coal feedstock
24	Pure EcoFuel (July 22, 1980)	27-005	XAD-2 resin
		27-011	Combined cyclones
		27-017	Particulate filter
		27-023	Organic trap condensate
		27-029	Fly ash
		27-035	EcoFuel feedstock
17	50 Percent EcoFuel/ 50 Percent Coal (May 23, 1980)	27-001	XAD-2 resin
		27-007	Combined cyclones
		27-013	Particulate filter
		27-019	Organic trap condensate
		27-025	Fly ash
		27-035	EcoFuel feedstock
		27-036	Coal feedstock

TABLE 6 (CONT.)

RUN ID	FLUIDIZED-BED FEEDSTOCK	ERCO LAB ID	SAMPLE
25	EcoFuel/Toluene (August 7, 1980)		
		27-006	XAD-2 resin
		27-012	Combined cyclones
		27-018	Particulate filter
		27-024	Organic trap condensate
		27-030	Fly ash
		27-035	EcoFuel feedstock
23	50 Percent MSW/50 Percent Coal (June 27, 1980)		
		27-004	XAD-2 resin
		27-010	Combined cyclones
		27-016	Particulate filter
		27-022	Organic trap condensate
		27-028	Fly ash
		27-034	MSW feedstock
		27-036	Coal feedstock

TABLE 7

PRELIMINARY ANALYSIS OF TOTAL EXTRACTABLE ORGANIC (TEO) CONTENT

RUN I.D.	ERCO LAB I.D.	TYPE OF SAMPLE	TCO (mg)	GRAV (mg)	TCO and GRAV (mg)	TEO (mg/g)
17	27-001	XAD-2 Resin	283.69	410.90	694.59	19.04
18	27-002	XAD-2 Resin	182.24	370.60	552.84	9.72
22	27-003	XAD-2 Resin	0.601	7.6	8.201	0.22
23	27-004	XAD-2 Resin	0.557	31.003	31.56	0.82
24	27-005	XAD-2 Resin	5.93	29.7	35.63	1.80
25	27-006	XAD-2 Resin	72.84	225.90	328.74	8.89
17	27-007	Combined Cyclones	0.215	12.19	12.4	1.11
18	27-008	Combined Cyclones	0.0398	19.00	19.04	2.48
22	27-009	Combined Cyclones	0.03	3.10	12.13	1.08
23	27-010	Combined Cyclones	5.096	4.8	9.896	1.16
24	27-011	Combined Cyclones	8.71	5.0	13.71	1.18
25	27-012	Combined Cyclones	7.61	6.3	13.91	1.29
17	27-013	Particulate Filter	0.873	42.83	43.70	11.69
18	27-014	Particulate Filter	7.48	135.1	142.58	37.13
22	27-015	Particulate Filter	6.49	2.0	8.49	2.53
23	27-016	Particulate Filter	4.43	2.30	6.73	2.90
24	27-017	Particulate Filter	11.96	3.0	14.96	31.17
25	27-018	Particulate Filter	6.07	7.4	13.47	19.81
17	27-019	Condensate	0.317	9.703	10.02	1.00
18	27-020	Condensate	5.425	5.71	11.13	0.192
22	27-021	Condensate	1.34	32.46	33.80	0.064
23	27-022	Condensate	10.59	18.91	29.5	0.059
24	27-023	Condensate	0.824	6.60	7.42	0.021
25	27-024	Condensate	305.43	882.6	1188.03	1.773

TABLE 7 (CONT.)

RUN I.D.	ERCO LAB I.D.	TYPE OF SAMPLE	TCO (mg)	GRAV (mg)	TCO and GRAV (mg)	TEO (mg/g)
17	27-025	Fly Ash	7.542	--	7.542	0.754
18	27-026	Fly Ash	6.81	2.4	9.21	1.25
22	27-027	Fly Ash	8.21	17.2	25.41	3.63
23	27-028	Fly Ash	6.39	38.5	44.89	7.48
24	27-029	Fly Ash	4.503	30.6	35.10	5.294
25	27-030	Fly Ash	0.1623	25.24	25.40	1.019
23	27-034	MSW Feed Stock	0.192	243.20	243.40	39.39
	27-035	EcoFuel Feed Stock	0.348	158.65	159.00	35.65
23	27-036	Coal Feed Stock	1.4	16.9	18.3	0.33

TABLE 8

ORGANIC CONTENT OF LC FRACTIONS

ERCO I.D.	TYPE OF SAMPLE	TCO (mg)	GRAV (mg)	TCO and GRAV (mg)	CONCENTRATION (mg/g)
27-001	XAD-2 Resin				
F_1	XAD-2 Resin	0.675	0.42	1.095	0.03
F_2	XAD-2 Resin	0.05	0.34	0.39	0.011
F_3	XAD-2 Resin	329.441	5.43	334.871	9.18
F_4	XAD-2 Resin	1.241	0.26	1.501	0.0412
F_5	XAD-2 Resin	3.291	0.81	4.111	0.1127
F_6	XAD-2 Resin	76.051	2.88	78.931	2.164
F_7	XAD-2 Resin	--	0.23	0.23	0.0063
27-002	XAD-2 Resin				
F_1	XAD-2 Resin	--	0.27	0.27	0.0048
F_2	XAD-2 Resin	13.73	0.05	13.78	0.2423
F_3	XAD-2 Resin	67.331	6.42	73.751	1.297
F_4	XAD-2 Resin	0.849	0.47	1.319	0.0232
F_5	XAD-2 Resin	2.158	0.46	2.618	0.0460
F_6	XAD-2 Resin	9.201	2.39	11.591	0.204
F_7	XAD-2 Resin	--	0.25	0.25	0.0044
27-006	XAD-2 Resin				
F_1	XAD-2 Resin	0.197	0.45	0.647	0.0175
F_2	XAD-2 Resin	0.088	0.16	0.248	0.0067
F_3	XAD-2 Resin	15.076	0.55	15.626	0.4223
F_4	XAD-2 Resin	0.190	0.29	0.48	0.0130
F_5	XAD-2 Resin	3.063	0.27	3.333	0.0901
F_6	XAD-2 Resin	45.737	3.82	49.667	1.3394
F_7	XAD-2 Resin	--	1.61	1.61	0.0435
27-024	Condensate				
F_1	Condensate	0.017	--	0.017	0.00025
F_2	Condensate	0.009	--	0.009	0.00013
F_3	Condensate	--	--	--	--
F_4	Condensate	0.007	--	0.007	0.0001
F_5	Condensate	15.85	0.67	16.52	0.0247
F_6	Condensate	21.249	25.80	47.049	0.0702
F_7	Condensate	4.919	0.37	5.289	0.0079

TABLE 8 (CONT.)

ERCO I.D.	TYPE OF SAMPLE	TCO (mg)	GRAV (mg)	TCO and GRAV (mg)	CONCEN-TRATION (mg/g)
27-034	MSW Feed Stock				
F_1	MSW Feed Stock	--	--	--	--
F_2	MSW Feed Stock	0.01	--	0.01	0.0016
F_3	MSW Feed Stock	--	2.85	2.85	0.4612
F_4	MSW Feed Stock	0.015	0.88	0.895	0.1448
F_5	MSW Feed Stock	--	--	--	--
F_6	MSW Feed Stock	--	2.23	2.23	0.3608
F_7	MSW Feed Stock	--	--	--	--
27-035	EcoFuel Feed Stock				
F_1	EcoFuel Feed Stock	0.923	0.91	1.833	0.4110
F_2	EcoFuel Feed Stock	0.233	--	0.233	0.0522
F_3	EcoFuel Feed Stock	--	0.24	0.24	0.0538
F_4	EcoFuel Feed Stock	0.004	0.12	0.124	0.0278
F_5	EcoFuel Feed Stock	--	0.17	0.17	0.381
F_6	EcoFuel Feed Stock	--	3.33	3.33	0.7466
F_7	EcoFuel Feed Stock	--	0.07	0.07	0.0157
27-036	Coal Feed Stock				
F_1	Coal Feed Stock	--	2.3	2.3	0.042
F_2	Coal Feed Stock	--	0.3	0.3	0.005
F_3	Coal Feed Stock	--	8.8	8.8	0.159
F_4	Coal Feed Stock	--	6.3	6.3	0.114
F_5	Coal Feed Stock	--	2.0	2.0	0.036
F_6	Coal Feed Stock	--	1.3	1.3	0.023
F_7	Coal Feed Stock	--	8.0	8.0	0.144

TABLE 9

GC/MS IDENTIFICATION AND QUANTIFICATION

COMPOUND	MW	CHARACTERISTIC IONS 1°m/e	2°m/e	3°m/e	CONCENTRATION (ug/g)
Sample 27-001 Fraction 1					
n-C_{14} alkane	198	57	71	85	12
n-C_{15} alkane	212	57	71	85	12
n-C_{16} alkane	226	57	71	55	18
n-C_{17} alkane	240	57	71	55	8
n-C_{18} alkane	254	57	71	85	12
n-C_{19} alkane	268	57	71	85	7
n-C_{20} alkane	282	57	71	85	9
hexasulfur	192	64	192	66	12
octasulfur	256	64	128	96	30
Sample 27-001 Fraction 2					
Cycloocta-tetraene	104	104	78	103	240
Indene	116	116	115	63	520
Naphthalene	128	128	129	127	4600
2-methyl naphthalene	142	141	142	115	340
1-methyl naphthalene	142	142	141	115	280
biphenyl	154	154	153	152	340
acenaphthene	154	154	153	152	210
acenaphthylene	152	152	151	150	1000
phenanthrene/ anthracene	178	178	200	201	100
pyrene	202	202	200	201	100

TABLE 9 (CONT.)

COMPOUND	MW	CHARACTERISTIC IONS			CONCENTRATION (ug/g)
		1°m/e	2°m/e	3°m/e	
Sample 27-001 Fraction 3					
Indene	115	115	116	63	400
Naphthalene	128	128	129	126	3400
Methyl naphthalene	142	142	141	115	280
Biphenyl	154	154	153	152	550
Acenaphthene	154	154	153	152	200
Acenaphthylene	152	152	151	150	1600
Dibenzofuran	168	168	139	63	430
Fluorene	165	165	166	82	380
Phenathrene	178	178	176	179	1100
Fluoranthene	202	202	200	203	280
Pyrene	202	202	101	200	300
Sample 27-001 Fraction 4					
Cyanobenzene	103	103	76	50	62
Naphthalene	128	128	127	129	690
Methyl naphthalene	141	141	142	115	62
Biphenyl	154	154	153	76	62
Acenaphthylene	152	152	76	151	280
Beta-naphthonitrile	153	153	126	154	250
Dibenzofuran	168	168	139	169	76
Flouorene	165	165	166	82	51
Phenanthrene	178	178	176	179	21
Fluoranthene	202	202	201	200	41
Pyrene	202	202	101	100	37

TABLE 9 (CONT.)

COMPOUND	MW	CHARACTERISTIC IONS 1°m/e	2°m/e	3°m/e	CONCENTRATION (ug/g)
Sample 27-001 Fraction 5					
Cyanobenzene	103	103	63	76	1000
Beta-naphthonitrile	153	153	126	154	270
4,4'-dipyridyl and 2,2'-dipyridyl	156	128	156	127	310
1-naphthyl-isocyanide	153	153	154	126	360
Phthalate	149	149	71	55	120
Sample 27-001 Fraction 6					
Benzaldehyde	105	77	105	106	1600
Phenol	94	94	66	65	2300
Salicylaldehyde	122	122	121	65	330
Cresol and Tolualdehyde	120	107	91	108	360
o-methoxyphenol	109	109	124	81	360
Benzoic acid	105	105	77	122	330
Phenyl-1-naphthloate	248	127	156	155	360
Fluorenone	180	180	152	151	1200
Benzo(c) cinnoline	180	152	180	151	260
Sample 27-001 Fraction 7					
o-nitrobenzoic acid	65	65	58	77	11
Benzoic acid	77	77	122	105	54

TABLE 9 (CONT.)

COMPOUND	MW	CHARACTERISTIC IONS 1°m/e	2°m/e	3°m/e	CONCENTRATION (ug/g)
Sample 27-002 Fraction 2					
Xylene	106	91	106	105	41
Cycloocta-tetraene	104	104	78	103	120
Cyclopropyl benzene	117	117	118	91	47
Indene	116	116	115	89	120
Naphthalene	128	128	127	129	900
Benzothiophene	134	134	89	135	110
2-methyl naphthalene	142	142	141	115	380
1-methyl naphthalene	142	142	141	115	110
Acenaphthylene	152	152	151	76	100
Sample 27-002 Fraction 3					
Indene	116	116	115	89	67
Naphthalene	128	128	129	127	400
Methyl naphthalene	142	142	141	115	81
Biphenyl	154	154	153	152	59
Acenaphthylene	152	152	151	150	200
Dibenzofuran	169	168	139	169	110
Fluorene	166	165	166	164	58
Phenanthrene	179	178	176	179	45
Fluoranthene	202	202	200	203	45
Pyrene	202	202	200	101	59

TABLE 9 (CONT.)

		CHARACTERISTIC IONS			
COMPOUND	MW	1°m/e	2°m/e	3°m/e	CONCENTRATION (ug/g)
Sample 27-002 Fraction 4					
Cyanobenzene	103	103	76	50	2900
Tolunitrile isomer	117	117	116	90	720
Tolunitrile isomer	117	117	90	116	790
1-methyl naphthalene	142	142	141	115	720
Biphenyl	154	154	152	76	860
Acenaphthene	152	152	151	150	1900
1-naphthyl-isocyanide	153	153	126	154	9600
B-naphtho-nitrile	153	153	126	154	1220
Carbazole	167	167	83	166	3700
Fluoranthene	202	202	100	101	720
Pyrene	202	202	203	101	790

TABLE 9 (CONT.)

COMPOUND	MW	CHARACTERISTIC IONS 1°m/e	 2°m/e	 3°m/e	CONCENTRATION (ug/g)
Sample 27-002 Fraction 5					
Benzaldehyde	105	77	105	106	34
Cyanobenzene	103	103	76	50	300
Tolunitrile isomer	117	117	90	116	97
Tolunitrile isomer	117	117	116	90	49
Tolunitrile isomer	117	117	116	90	50
Naphthalene	128	128	129	102	58
B-naphthonitrile	153	153	126	63	310
Sample 27-002 Fraction 6					
Benzeldehyde	106	105	106	77	450
Phenol	94	94	66	65	2900
p-cresol	108	108	107	77	260
1,2-naphthaquinone	158	130	102	50	190
Quinoline	129	129	102	128	410
2,2'bipyridyl	156	156	127	155	240
1,2,4-trichlorobenzene	180	180	152	151	990
Benzo(c)cinnoline	181	152	180	151	890
Anthraquinone	208	208	180	152	280
Phthalate	263	149	263	133	190
Benzanthrone	230	230	202	201	190

TABLE 9 (CONT.)

COMPOUND	MW	CHARACTERISTIC IONS 1°m/e	CHARACTERISTIC IONS 2°m/e	CHARACTERISTIC IONS 3°m/e	CONCENTRATION (ug/g)
Sample 27-006 Fraction 1					
Dichlorobenzene isomer	146	146	148	74	16
Dichlorobenzene isomer	146	146	75	146	13
Trichlorobenzene isomer	182	180	182	74	70
Trichlorobenzene isomer	182	182	180	74	29
Bromodichlorobenzene	226	74	226	109	16
Tetrachlorobenzene isomer	216	216	214	218	20
Tetrachlorobenzene isomer	216	216	214	217	22
n-C_{12} alkane	170	71	57	85	14
n-C_{14} alkene	196	55	57	69	13
n-C_{14} alkane	198	57	71	85	22
n-C_{15} alkene	210	55	83	69	20
n-C_{16} alkene	224	55	69	57	16
n-C_{17} alkene	238	55	69	57	11
n-C_{18} alkene	252	55	69	57	11
n-C_{19} to u-C_{23} alkanes or alkenes present in low concentrations.					
n-C_{24} alkane	338	57	71	69	13
n-C_{25} alkane	352	57	71	85	13
n-C_{26} alkane	366	57	71	85	16
n-C_{27} alkane	380	57	71	85	23
n-C_{28} to u-C_{31} alkanes present in low concentrations.					

TABLE 9 (CONT.)

COMPOUND	MW	CHARACTERISTIC IONS 1°m/e	2°m/e	3°m/e	CONCENTRATION (ug/g)
Sample 27-006 Fraction 3					
Naphthalene	128	128	127	127	1400
Methyl naphthalene	142	142	141	115	620
Biphenyl	154	154	153	152	12650
Methyl biphenyl	167	167	168	165	520
Acenaphthene	152	152	76	151	1100
Diphenyl-methane	168	168	167	165	720
Dibenzofuran	169	168	139	91	2500
Fluorene	167	166	165	167	610
Dihydro-phenanthrene	180	180	179	89	2600
Terphenyl isomer	230	230	229	215	720
Terphenyl isomer	242	230	231	115	1100
Terphenyl isomer	230	230	231	228	820
Sample 27-006 Fraction 4					
Chlorophenol	128	128	63	64	170
Benzoyl chloride	105	105	77	51	1000
Dichlorophenol	162	162	164	63	130
Biphenyl	154	154	153	152	120
Benzoic anhydride	122	105	122	77	120
Phenyl diphenyl-4-carboxylate	181	181	152	153	94

TABLE 9 (CONT.)

COMPOUND	MW	CHARACTERISTIC IONS 1°m/e	 2°m/e	 3°m/e	CONCENTRATION (ug/g)
Phenyl diphenyl-4-carboxylate	181	181	152	153	380
Methyl decanoate	87	74	87	55	110
Sample 27-006 Fraction 5					
p-chloro phenol	128	128	130	63	1700
Thiobenzoic acid	105	77	105	51	4000
Ethyl benzoate	150	77	105	51	11000
Methyl benzoate	136	105	77	51	2700
Fluorenone	180	180	152	151	820
Sample 27-006 Fraction 6					
Phenol	94	94	66	65	3200
Acetophenone	120	105	77	120	1200
Methyl benzoate	136	105	77	51	1300
Benzoic acid	122	105	77	122	3700
Ethyl benzoic acid	150	105	150	135	760
Allyl benzoate	162	195	77	123	2400
Benzophenone	182	105	182	77	1700
Fluorenone	181	180	152	151	2900
Nitro-benzophenone	167	105	77	51	5900

TABLE 9 (CONT.)

COMPOUND	MW	CHARACTERISTIC IONS 1°m/e	2°m/e	3°m/e	CONCENTRATION (ug/g)
Sample 27-024 Fraction 5					
Benzaldehyde	106	106	77	105	64
Methyl benzoate	136	105	77	136	46
Benzoic acid	122	105	77	122	600
Methyl benzoic acid	136	91	136	119	46
Chlorobenzoic acid	156	156	139	111	40
Ethyl benzoic acid	150	105	135	77	72
Benzophenone	182	105	77	182	100
Fluorenone	180	180	152	151	40
Nitrobenzoic acid	167	105	77	51	40
Sample 27-024 Fraction 6					
Phenol	94	94	66	65	2800
Benzoic acid	123	105	77	122	13000
p-methyl benzoic acid	136	91	136	119	1400
p-chloro benzoic acid	156	139	156	111	500
o-chloro benzoic acid	156	139	156	50	1000
Isobutyl cinnamate	204	148	131	77	1000
Isopropyl benzoate	164	105	77	123	4400

TABLE 9 (CONT.)

COMPOUND	MW	CHARACTERISTIC IONS 1°m/e	 2°m/e	 3°m/e	CONCENTRATION (ug/g)
Sample 27-024 Fraction 7					
Phenol	94	94	66	65	110
Benzoic acid	122	105	77	122	540
p-methyl benzoic acid	136	91	119	136	28
Benzamide	121	105	77	121	74
Isopropyl benzoate	164	105	77	123	130
Sample 27-034 Fraction 3					
Acetophenone	120	105	77	120	19
Cumene	120	105	120	77	49
Naphthalene	128	128	77	51	29
Sample 27-034 Fraction 6					
Benzoic Acid	122	105	77	122	69
Nonanoic acid	158	60	73	57	34
Isophthalic acid	166	149	91	104	43
Dicyclohexyl-phthalate	330	149	55	167	62
Bis (2-ethyl hexyl) phthalate	390	149	167	279	200

TABLE 9 (CONT.)

COMPOUND	MW	CHARACTERISTIC IONS 1°m/e	2°m/e	3°m/e	CONCENTRATION (ug/g)
Sample 27-035 Fraction 1					
n-C_{18} alkane	254	58	64	-	180
n-C_{19} alkane	268	85	69	77	220
n-C_{20} alkane	282	57	55	67	180
n-C_{21} alkane	296	71	57	85	320
n-C_{22} alkane	310	57	55	71	970
n-C_{23} alkane	324	57	55	71	1260
n-C_{24} alkane	338	57	71	85	1260
n-C_{25} alkane	352	57	55	71	1550
n-C_{26} alkane	366	57	71	85	1100
n-C_{27} alkane	380	57	55	71	936
n-C_{28} alkane	394	57	71	55	860
n-C_{29} alkane	408	57	71	55	430
n-C_{30} alkane	422	57	71	69	400
n-C_{31} alkane	436	57	71	69	290
Sample 27-035 Fraction 6					
Biphenyl	152	152	151	81	940
Nonanoic acid	158	60	73	55	720
Bis (2-ethyl hexyl) phthalate	320	149	167	279	5200

TABLE 9 (CONT.)

COMPOUND	MW	CHARACTERISTIC IONS 1°m/e	2°m/e	3°m/e	CONCENTRATION (ug/g)
Sample 27-009 Total Extract					
Naphthalene	128	128	129	127	4060
2-chloro-naphthalene	162	162	127	164	420
Dibenzofuran	168	168	139	169	260
Sample 27-010 Total Extract					
Xylene	106	91	106	105	190
Benzoic acid	105	105	77	122	320
Naphthalene	128	128	51	127	2,500
Biphenyl	154	154	153	152	440
Coumarin	146	118	146	89	150
Dibenzofuran	168	168	139	84	210
Fluorenene	180	180	152	151	150
Phenanthrene	178	178	176	179	180
Sample 27-011 Total Extract					
Phenol	94	94	66	65	68
Benzoic acid	106	105	77	122	140
Phthalate	-	71	149	55	100
Diisobutyl phthalate	390	149	57	76	44

TABLE 9 (CONT.)

COMPOUND	MW	CHARACTERISTIC IONS			CONCENTRATION (ug/g)
		1°m/e	2°m/e	3°m/e	
Sample 27-012 Total Extract					
n-C_{14} alkane	198	57	71	85	58
n-C_{15} alkane	212	57	71	55	37
n-C_{16} alkane	226	57	71	56	46
n-C_{17} alkane	240	57	71	55	46
Phenyl benzoate	182	105	77	51	58
Sample 27-014 Total Extract					
Xylene/ethyl benzene	106	91	106	105	38
Benzoic acid	122	105	77	122	27
Naphthalene	128	128	129	127	90
Anthracene/ phenanthrane	178	178	176	152	63
Fluoranthene	202	202	200	203	14
Pyrene	202	202	101	100	23
3,4-benzo-phenanthrene	226	226	228	227	45
Benzo(a)-anthracene	228	228	226	229	18
Chrysene	228	228	226	229	33
Benzanthrene	230	230	202	200	18
Benzo(b)-fluoranthene	252	252	125	250	27
Benzo(k)-fluoranthene	252	252	268	250	11
Benzo(e)-pyrene	252	252	253	250	14

TABLE 9 (CONT.)

COMPOUND	MW	CHARACTERISTIC IONS			CONCENTRATION (ug/g)
		1°m/e	2°m/e	3°m/e	
Benzo(a)pyrene	252	252	254	253	29
Perylene	252	252	126	125	6
Sample 27-020 Total Extract					
2-methylpyridine	93	93	66	92	380
phenol	94	94	66	65	2,700
p-cresol	108	107	108	77	380
1,2 dicyanoethyelene	78	131	78	103	200
Isoquinoline	129	129	102	128	1,900
Quinoline	129	129	128	102	640
2-methyl quinoline	143	149	128	115	400
8-methyl quinoline	143	143	142	115	200

TABLE 9 (CONT.)

		CHARACTERISTIC IONS			
COMPOUND	MW	1°m/e	2°m/e	3°m/e	CONCENTRATION (ug/g)
Sample 27-021	Total Extract				
2-methyl furan	82	82	53	96	330
2-vinyl furan	94	94	65	66	210
Anthracene/ phenanthrene	178	178	176	76	530
Benzo(c)-cinnoline	152	152	192	180	150
Dibenzo-heptafulvene	204	204	202	203	160
Fluoranthene	202	202	101	200	680
Pyrene	202	202	200	201	2,900
3,4-benzo-phenanthrene	226	226	227	228	160
9,10-benzo-phenanthrene	226	228	226	229	210
16,11-benzo-fluoranthene	252	252	253	250	120

TABLE 9 (CONT.)

		CHARACTERISTIC IONS			
COMPOUND	MW	1°m/e	2°m/e	3°m/e	CONCENTRATION (ug/g)
Sample 27-022 Total Extract					
Isophorone	136	82	96	95	580
2,4-dimethyl furan	96	96	67	53	170
2-formyl-imidazole	96	68	96	50	220
Phenol	94	94	66	65	2,100
p-cresol	108	108	107	77	170
o-cresol	108	107	108	77	760
2-methyl hydroquinone	124	124	123	95	360
Nitroso-benzene	107	77	107	51	220
Benzoic acid	105	105	77	122	950
1,3 dicyano-benzene	128	128	101	75	160
Vanillin	152	151	152	81	290

TABLE 9 (CONT.)

COMPOUND	MW	CHARACTERISTIC IONS 1°m/e	 2°m/e	 3°m/e	CONCENTRATION (ug/g)
Sample 27-023 Total Extract					
Phenol	94	94	66	65	760
Benzoic acid	105	105	77	122	350
Chlorophenol	128	128	130	65	220
1,2 cyano-ethylene	78	78	51	131	140
Isoquinoline	108	129	102	128	190
Bromophenol	173	172	65	174	100
Phthalide	134	105	77	134	110
Chromone	146	146	118	92	86
Coumarin	146	118	146	89	210
Phthalimide	147	147	76	104	370
4,4'dipyridyl	156	156	127	64	100
Fluorenone	180	180	152	151	150
Acenaphthene	154	154	126	182	120
Benzo(c)-cinnoline	152	152	180	151	440
Diethyl-phthalate	222	149	150	104	86
9,10-anthra-quinone	208	152	208	180	100
Acenaphthene	154	154	126	198	520

TABLE 10

ORGANIC EMISSION RATES (mg TEO/lb feedstock)[a]

Run ID	17	18	22	23	24	25
Run Date	5/23	5/28	6/24	6/27	7/22	8/7
Feedstock Composition (wt %)						
Coal/Eco/MSW/ Toluene	50/50/0/0	100/0/0/0	100/0/0/0	50/0/50/0	0/100/0/0	0/82/0/18
Bed Temperature (° F)	1500	1500	1250	1250	1500	1550
TEO Emission (mg TEO/lb feedstock)						
Feedstock[b]	8167	150	150	9016	16185	94000
Reactor fly ash	34	86	220	480	236	37.3
Combined cyclones[c]	6.54 (1.3%)	33.2 (7.3%)	14.50 (NA)	9.87 (35.5%)	5.06 (18.4%)	4.84 (1.8%)
Particulate filter[c]	9.04 (1.8%)	59 (13.0%)	2.60 (NA)	1.28 (4.6%)	2.71 (9.8%)	3.51 (1.3%)
XAD-2 Resin[c]	297 (60.5%)	343 (75.5%)	5.08 (NA)	11.8 (42.7%)	17.3 (62.8%)	109.3 (41.0%)
O.M. Condensate[c]	178 (36.3%)	19.0 (4.2%)	NA (NA)	4.78 (17.2%)	2.46 (8.9%)	148.9 (55.8%)
Total[d]	524	540	242+	508	263	304

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[a] TEO is the last column in Table 7 defined as total extractable organic content.

[b] Calculated by weighting feedstock according to weight percent.

[c] The percentage values exclude the reactor fly ash samples. Percentage of organic collected by SASS alone.

[d] Excludes feedstock TEO.

VI. Discussion of Results

A. Combustion Issues

Referring to the summary Table 4 for the ERCO Pilot Plant Tests, it is apparent that the carbon burn-out efficiency (carbon in flue gas/carbon in feedstock) ranged from 93 to 98 percent; these values are accurate to within 10 percent because of the inability to meter the feed more precisely (particularly with the MSW).

The fluidization velocity was about 4.4 fps (at 1500 °F) for the 50/50:Coal/EcoFuel Run (#17) and the 100/0:Coal/Ecofuel Run (#18). There was more above-the-bed burning with Run #17 (as evidenced by the difference between the lower freeboard and bed temperatures), which is attributable to the fine size of the EcoFuel feedstock.

It is noted that the pure EcoFuel Run #24 had freeboard burning comparable to Runs 17 (50/50:Coal/EcoFuel) and 18 (100/0:Coal/EcoFuel). The reason for this is that this run was performed at a reduced fluidization velocity (2.8 fps vs. 4.4 fps). Investigators have shown that elutriation is proportional to the 3rd or 4th power of the excess velocity (actual fluidization minus minimum fluidization velocity).

When the bed temperature was reduced to 1250° F with coal (Run #22), excessive freeboard burning was evidenced in the trial runs. For this reason the fluidization velocity was reduced to 2.7 fps. Increased freeboard burning is due to reduced reaction rates at reduced bed temperatures.

The runs were not performed with the same excess air (variation from 35 to 59 percent) because of the desire to maintain a minimum fluidization velocity and the variation in the feedrate over the course of the run.

The overall heat balance (Q out/Q in) was reasonable (0.80-0.93) for Runs 17, 18, and 25. For the runs at the lower bed temperature (22 and 23) and the run with pure EcoFuel (24), the overall heat balance was poor. This is attributed to the fact that steam was formed in the in-bed cooling water tubes, which made this heat output term somewhat tenuous.

B. SASS Train Results (Refer to Table 5)

The majority (>90 percent) of the particulate was collected in the SASS cyclones; even so the particulate leading to the filter still required 3 to 5 filter changes in order to maintain a minimum sampling rate of 2.7 DSCFM.

The amount of liquid collected in the O.M. condensate trap varied considerably from run to run and the magnitude of this value is somewhat tenuous.

The normalized rates of emissions (g material/lb feedstock) were calculated from the procedure described in Section V A.

C. Organic Analysis - Level 1 Results

A review of Table 7 indicates that a majority of the RDF combustion samples contain relatively low amounts of characterizable organics. The values for the sum of the gravimetric data and TCO were used to determine whether there was an adequate quantity of organics present to employ the column chromatography fractionation scheme and subsequent GC/MS analysis. A summary of the relative quantities of organics present in the RDF samples is illustrated in Table 11. Regardless of organic content, all feedstock extracts were fractionated and analyzed so as to provide background information for data interpretation.

Substantial quantities of organics were generally found only in the XAD-2 resin, which was used to filter the combustion vapor. Recently a comprehensive review of organic emissions from selected combustion processes was published by Junk and Ford (1980). Interestingly, quite a few of the organics identified here have previously not been detected in combustion effluents. A review of the organics found in each RDF combustion experiment follows.

Pure Coal Burned at 1500°F - Run #18

Although the chemical composition of coal has not been totally delineated, there has recently been an extensive effort in characterizing the organic content of coal (e.g., Schultz et al., 1979). However, the effort in characterizing organic emissions from coal combustion is considered inadequate (Junk and Ford, 1980). In terms of concentration, most of the organics detected in the combustion effluent of this burn resided on the XAD-2 resin, and to a lesser extent

TABLE 11

RELATIVE AMOUNTS OF ORGANICS IN SASS[a]

RUN ID	EXPERIMENT	XAD-2 RESIN	COMBINED CYCLONES	PARTICULATE FILTERS	TRAP CONDENSATE	FLY ASH
18	Pure Coal at 1500° F	A	B	B	B	B
22	Pure Coal at 1250° F	B	B	B	B	B
24	Pure EcoFuel	B	B	B	B	B
17	50% EcoFuel/ 50% Coal	A	B	B	B	B
25	EcoFuel/ Toluene	A	B	B	A	B
23	50% MSW/ 50% Coal	B	B	B	B	B

Key

A = Organics present in substantial quantities. Full Level 1 protocol used.
B = Organics present in relatively low concentration.

[a] Based on Table 7 results.

on the particulate filter. The fractionation scheme indicates organics to be present throughout the full polarity range for the XAD-2 resin extract. Polycyclic aromatic hydrocarbon (PAH) were the dominant organic compounds contained in the XAD-2 resin extract. This is not surprising since PAH are recognized constituents of coal (Schultz et al., 1979; White and Lee, 1980; Snape et al., 1979), as well as the byproduct of combustion processes (Laflamme and Hites, 1978) as has been demonstrated in industrial processes (e.g., Yu and Hites, 1981; Davies et al., 1976; Alsberg and Stenberg, 1979; Pederson et al., 1980; Serth and Hughes, 1980). This is of special interest since many PAH are known chemical carcinogens (Josephson, 1981), and many are considered by EPA (1979b) to be priority pollutants. Other chemical classes detected include some heterocyclic compounds, cyanoaromatics, phenols and oxygenated aromatics (e.g., benzaldehyde, anthraquinone). Compounds unique in the literature (as reported by Junk and Ford, 1980) include cyclooctatetraene, cyanobenzene, 1-naphthyl isocyanide, and benzaldehyde. The absence of cyanobenzene in the literature is surprising since many cyanoaromatics have been detected in combustion effluents (e.g., Krishman et al., 1979). The detection of dibenzofuran and biphenyl is interesting. Although their chlorinatd analogs were not detected (PCDF and PCB respectively), they may still be present in trace quantities because the mass spectrometer is not quite as sensitive to these classes of compounds. Both classes of compounds, especially PCDF, are regarded as toxic (Moore et al., 1976). A GC/MS screen was also performed on the total extract derived from the particulate filter. This sample contained PAH compounds of higher molecular weight than those seen in the XAD extract, such as benzofluoranthenes, benzopyrenes and perylene.

It should be noted that the Level 1 protocol does not dictate that samples with low levels of organics be analyzed by GC/MS. However it is evident that organics of undetermined structure are present in many of the other extracts, and very well may have toxic organic compounds present in them. For example, fly ash samples from municipal incincerators contain many trace organics such as polychlorinated dibenzofurans, polychlorinated dibenzo-p-dioxins (TCDD), polychlorinated benzenes, polychlorinated phenols, PAH, phthalate esters, and aliphatic hydrocarbons (e.g., Eiceman et al., 1979; 1981), some of which are known carcinogens. Therefore it may be advisable to examine some of the samples in more detail as a follow-up to this program.

Pure Coal Burned at 1250° F (Run #22)

The combustion of coal at lower temperatures than the preceding burn produced effluents with surprising lower organic content. This may be attributable to the reduced fluidizing velocity for this run compared to run #18. The only GC/MS analysis performed on this sample was the total extract from the organic trap condensate. PAH were again quite evident. A very unusual compound, dibenzoheptafulvene, was also detected. This compound has not yet been recorded in the literature (Junk and Ford, 1980) as being present in combustion emission. Its formation may occur through a rearrangement reaction requiring insertion of a carbon atom into an aromatic moiety.

Pure EcoFuel at 1500° F (Run #24)

The organic composition of the Eco refuse material was primarily aliphatic hydrocarbons, as well as trace quantities of organic acids and esters. After combustion, GC/MS analysis of the cyclone material and the organic trap condensate indicated significant quantities of phenol and benzoic acid were present. Both these compounds are likely oxidative degradation products of lignin (polymer of phenylpropanoids). Lignin is the main constituent of wood, and thus is present in the paper waste contained in the Eco refuse. Other compounds which may be indirectly generated from lignin include chlorophenol, bromophenol, phthalide, cumene and chromone. PAH compounds and a few nitrogen heterocyclic compounds were also present. The formation of PAH has been alluded to earlier in this section. Nitrogen heterocyclics, which were detected in the trap condensate, are also known to be found in combustion processes (Dong et al., 1977), and in some cases are suspected carcinogens (Arcis and Argus, 1974).

50 Percent EcoFuel/50 Percent Coal at 1500° F (Run #17)

A majority of the organic emittants produced from the combustion of this feedstock combination were contained on the XAD-2 resin. Quite a variety of compounds were detected in this extract. Compound classes include aliphatic hydrocarbons, PAH, heterocyclics, oxygenated aromatics and aromatic nitrites. Most of these compounds were originally present in the combusion effluent of either the pure coal or pure EcoFuel.

EcoFuel/Toluene at 1550° F (Run #25)

The addition of toluene to the Eco refuse generated a large number of benzene derivatives not seen in the combustion of pure EcoFuel. The list of new compounds includes bi-, tri-, and tetrachloro isomers of benzene, diphenyl methane, terphenyl isomers, benzoic acid esters and thiobenzoic acid. Trichlorobenzene is currently included on EPA's (1979b) priority pollutant list. Some alkylated PAH compounds were also unique to this combustion effluent, as well as some keto-aromatics (fluorene, benzophene, acetophenone).

50 Percent MSW/50 Percent Coal at 1250° F (Run #23)

The combination of MSW and coal seems to have generated lower quantities of organics in the SASS than the combination of EcoFuel (17) and coal. Qualitatively the MSW feedstock contained many of the same organic acids and acid derivatives present in the EcoFuel; however the large quantity of aliphatic hydrocarbons present in the Eco refuse was not present in the MSW. In regards to the combustion of MSW coal, all organics identified in the cyclones were similar to those identified in the Eco/coal burn. However, in the condensate there were many unique compounds identified, including isophorone, 2,4-dimethylfuran, 2-formylimidazole, 2-methyl hydroquinone, nitrobenzene, and 1,3-dicyanobenzene. Isophorone is currently listed as a priority pollutant by EPA (1979b).

It is noted that the concentration of the extractable organics was greater for the fine particulate captured on the SASS filter than for the particulate captured by either the reactor cyclone (fly ash) or the combined SASS cyclones.

D. Organic Emission Rates

Excluding the reactor fly ash samples, the results in Table 10 indicate that most (on a percentage basis) of the extractable organics from the SASS samples are collected on the XAD-2 resin or in the organic module condensate. In run #23 (50/50:Coal/MSW) at 1250° F, an unusually high percentage was collected by the combined SASS cyclones. This might be due to the reduced combustion temperature (1250° F vs. 1500-1550° F).

There does not appear to be any correlation between the total TEO emitted/lb feedstock compared with the TEO of the feedstock (average if a mixture employed).

Comparing the EcoFuel and coal runs (#18, 17, and 24 with 100, 50, and 0 percent coal, respectively) which were carried out at 1500° F, the emission data in Table 10 indicate that the amount of organics (per lb of feedstock) on the XAD-2 resin and O.M. condensate are definitely less for the run with the pure EcoFuel (Run #24).

With this limited run data, it is also not possible to quantify the effect of combustion temperature. One can compare run 18 (100% coal at 1500° F) and run 22 (100% coal at 1250° F) organic emissions (mg/lb) for the same SASS samples and there does not appear to be any trend. However, the fly ash from the reactor (refer to Table 7) for Run 22 does have a higher concentration of TEO compared to Run 18, which is what would be expected at reduced combustion temperatures. It is noted that run 22 was performed at a reduced fluidization velocity (2.7 fps) compared to run 18 (4.3 fps).

Comparing the toluene/EcoFuel run (Run #25) with the corresponding EcoFuel run (Run #24), which was performed at nominally the same combustion conditions, there were substantially more organic emissions per pound of feedstock associated with the XAD-2 resin and the O.M. condensate trap for Run #25 with toluene (refer to Table 10).

VII. Summary and Conclusions

1. Combustion efficiencies of 93 to 98 percent were achieved with the various coal/EcoFuel/MSW/toluene feedstock mixes in the 20-inch-diameter fluidized-bed reactor. Reaction temperatures ranged from 1250° to 1550° F and fluidization velocities ranged from 2.7 to 4.4 fps.

2. Most of the extractable organic emissions collected by the SASS train were collected on the XAD-2 resin and in the organic module condensate.

3. The extractable organic concentration of the particulate from the SASS train filter is higher than that of the reactor fly ash and the SASS combined cyclones.

4. There is no correlation between the total extractable organics emitted per pound of feedstock compared with the extractable organic content of the feedstock. However, the extractable organics collected by the XAD-2 resin and the O.M. condensate (per pound of feedstock) are clearly less for the pure EcoFuel run (#24) compared to the runs with either pure coal (#18) or 50/50:Eco/Coal (#17).

5. Reducing the coal combustion temperature from 1500° F (Run #18) to 1250° F (Run #22) increased the concentration of extractable organics in the reactor fly ash.

6. Addition of toluene to the EcoFuel did not increase the total organic emissions (per pound of feedstock), but did result in significantly more emissions

associated with the XAD-2 resin and the organic module condensate samples.

7. Polycyclic aromatic hydrocarbons (PAH) were the dominant organic compounds contained in the XAD-2 resin extract from the coal combustion run at 1500° F (Run #18).

8. In the combustion of pure EcoFuel at 1500° F (Run #24), reduced amounts of PAH compounds were found. Significant amounts of phenol and benzoic acid were identified.

9. The addition of toluene to the EcoFuel refuse generated a large number of benzene derivatives not seen in the combustion of pure EcoFuel. The list of new compounds includes bi-, tri-, and tetrachloro isomers of benzene.

VIII. Recommendations for Future Work

1. Investigate organic emission from combustion of a specific fuel at a number of different temperatures.

2. Perform trace metal analysis of a selected number of impinger samples collected from the ERCO runs.

3. Investigate the combustion of hazardous wastes other than toluene in an AFBC.

4. Provide for pneumatic injection of coal, EcoFuel and possibly MSW to provide a more accurate determination of the solid fuel feedrate. Also employ a weigh belt for solids metering.

APPENDIX I

IR SCREEN OF ORGANIC EXTRACTS

SAMPLE NO. 27-001

WAVE NO. CM^1	INTENSITY	INFERENCE
3150	M	-C = C-, -0H, NH-
3110	M	$C_6 4_6$, PARA, META, ORTHO-, Aromatics
3050	M	-Ch=CH, Napthalenes
3010	M	-C=C-H, Aromatics, Alkenes
1830	M	0=C-0-C=0, Alkenes
1810	M	C=C, Alkenes
1790	W	C=CH-; -C=0, Vinyl esters

SAMPLE NO. 27-002

WAVE NO. CM^1	INTENSITY	INFERENCE
3150	M	-C=C-, -0H, NH
3010	M	-C=C-H, Aromatics Alkenes
2950	W	-C-C-, Alkanes
2550	W	SH
2000	W	-C≡C-, Alkyne
1960	W	0=C-0-C=0
1800-1900	W	-C=0, -C00, esters

SAMPLE NO. 27-003

WAVE NO. CM^1	INTENSITY	INFERENCE
3500-2750	B	-COOH, Carboxylic acid
2700	W	$N-CH_3$, Amines
2600	W	SH, Sulfur
2420	W	N^+-H
2150	BW	$C=N^+-H$, $C\equiv C$
1830	BS	C=0, esters
1730	W	R-C-0-N, R-C-0-SH, -C00-, 0=C-C=0
1670	W	N-C=0, Lactam, A_r-COA_r, Quinones
1630	W	-C0-CH-0H, $CO-CH-NH_2$ C=C
1570	M	C=N, aromatic, N^+H, C=C, N=0
1500	M	C=C, N^+H, N=0
1400	W	C-H $(C0-CH_2)$, C-H(C=C-H)
1420	M	C=C, Aromatics
1300	BM	C-N, N-0 Aromatics
1150	M	C-0, C-0-C, C-N
1120	M	C-0, C0-C, CN
1020	M	C-0, C-0-C, CN
870	W	CH, N-H
800	M	CH, N-H
750	W	CH_2

SAMPLE NO. 27-004

WAVE NO. CM^1	INTENSITY	INFERENCE
3200-3700	BW	-OH; Carboxylic Acid
3150	W	-C=C-. -OH, NH
3050	S	$-CH=CH_2$, Napthalene
2980	W	-C-C-, Alkane
2800	W	N-C-H, $-O-CH_3$
2700	W	$N-CH_3$, Amines
2600	W	SH, Sulfur
1760	BS	-C=O, esters
1640	W	-CO-CH-OH, $CO-CH-NH_2$; C=C
1560	W	C=N, N^+H, C=C, N=O, Aromatics
1500	M	C=C, N^+H, N=O
1460	W	C=C Aromatics
1380	W	C-H, -OH
1320	M	C-N, NO_2 Aromatics
1260	M	C-N, NO_2
1220	W	C-O-C, $-CH_3$
1160	W	C-O, C-O-C, C-N
1050	W	C-O, C-O-C, C-N
870	W	CH, N-H
830	W	-CH, N-H
760	M	-CH, N-H
730	W	$-CH_2$

SAMPLE NO. 27-005

WAVE NO. CM^1	INTENSITY	INFERENCE
3030	BW	$H_2$0 (moisture)
1750	S	R-COO-N, R-COO-SH, -COO, 0=C-C=0
1640	M	C=C, -CO-CH-0H, CO-CH-NH_2
1460	W	C=C, Aromatic
1430	W	C=C
1230	W	C-0-C, C-H
860	W	CH, N-H
820	W	CH, N-H
780	M	CH_2

SAMPLE NO. 27-006

WAVE NO. CM^{1}	INTENSITY	INFERENCE
2900-3630	BS	-0H, Carboxylic acids
2700	M	N-CH$_3$, Amines
2650	W	SH, Sulfur
2050	W	-C≡C-
1970	W	0=C-0-C=0
1750	S	C=0, -C00
1670	M	N-C=0, A$_r$-C-O-A$_r$ 0=C=0 Quinone
1640	M	-C-0-CH-0H, C-0-CH-NH$_2$, C=C
1540	W	C=N, Aromatic, N$^+$H, C=C, N=0
1510	M	C=C, N$^+$H, N=0
1400	S	C-H(C0-CH$_2$), C-H(C=CH)
1370	M	C-H, -0H
1300	S	C-N, N-0; aromatics
1230	S	C-0-C, -CH$_3$
1180	S	C-0, C-0-C, C-N
1140	S	C-0. C-0-C, C-N
1110	S	C-0, C-0-C, C-N
1050	S	C-0, -C-0-C-, CN
1000	W	C-0. -C-0-C-, CN
960	S	N-0, C-H
860	M	CH, N-H
830	W	CH, N-H
800	W	N-H, CH, CH$_2$
780	M	CH, C=C-H
750	S	CH, C=C-H
710	M	CH$_1$ C=C-H
700	S	CH$_2$, CH$_1$, CN
680	W	CH$_2$, CH, CN

SAMPLE NO. 27-007

WAVE NO. CM^1	INTENSITY	INFERENCE
3150	W	-C=C-, -OH, NH_2
3000	W	-C=C-H, Aromatics, Alkenes
1760	W	C=O
1650	W	-CO-CH-OH, CO-CH-NH_2, C=C
1470	W	C=C, aromatics
940	W	N-O, C-H
870	W	CH, N-H
800	M	N-H, CH, CH_2

SAMPLE NO. 27-008

WAVE NO. CM^1	INTENSITY	INFERENCE
750	W	CH, C=C-H

SAMPLE NO. 27-009

WAVE NO. CM^{1}	INTENSITY	INFERENCE
2970	W	-C-C-, alkanes
2900	W	-C-C, alkanes
2850	W	C-H, $\mathrm{O-CH_3}$
2800	W	N-C-H, $\mathrm{-O-CH_3}$
2300	W	P-H, $\mathrm{N^{+}-H}$

SAMPLE NO. 27-011

WAVE NO. CM^1	INTENSITY	INFERENCE
2920	M	CH, N^+-N
2680	W	OH...O
2350	W	P-H, N^+-H
1450	W	C=C, aromatic
1370	W	C-H, OH
1270	W	CN, NO_2
750	W	CH, N-H
710	W	$-CH_2$

SAMPLE NO. 27-012

WAVE NO. CM^1	INTENSITY	INFERENCE
3050	W	$-C=CH_2$; napthalenes
2900	M	-C-C, alkane
2600	W	SH, sulfur
2350	W	P-H, N ± H
1710	W	R-COO-N, R-COOSH,-COO, O=C-C=0
1620	W	$-CO-CH-OH_1$ $CO-CH-NH_2$, C=C
1470	W	-C=C, aromatic
1380	W	-C-H, -OH
1300	W	-C-N, NO; aromatics
1250	W	-C-N, NO_2
740	W	$-CH_2$
700	W	$-CH_2$

SAMPLE NO. 27-013

WAVE NO. CM^{1}	INTENSITY	INFERENCE
3050	M	-CH=CH$_2$, Napthalene
2980	W	-C-C-; alkane
2910	M	-C-C-; alkane
2880	W	CH, OH...0, O-CH$_3$
2340	W	P-H, N+-H
1730	W	R-COO-N, R-COO-SH, -COO, O=C-C=0
1620	BM	-CO-CH-0H, CO-CH-NH$_2$ C=C
1410	W	C-H(CO-CH$_2$), C-H(C=C-H)
1260	M	C-N, NO$_2$
1070	W	C-O, C-O-C, CN
1030	W	C-O, -C-O-C, CN
880	M	CH, N-H
820	M	CH, N-H
750	M	CH C=C-H
660	W	CH$_2$ CH$_1$ CN

SAMPLE NO. 27-014

WAVE NO. CM^{1}	INTENSITY	INFERENCE
3050	M	$-CH=CH_2$, napthalenes
2950	W	-C-C-, alkanes
2350	W	$P-H_1$ N^+H
2120	W	$C=N^+-H$ C C
2040	W	$-C\equiv C-$
1920	W	C=0, N^+H
1820	W	C=0, $0=C-C=0_1$ C=C
1720	M	R-COO-N, R-COO-SH, - COO 0=C-C=0
1600	M	C=C, N-H,, C=0
1450	M	C=C, aromatics
1370	W	C-H, -OH
1270	W	CN, NO_2
1170	W	C-O, C-O-C, C-N
1070	W	C-O, C-O-C, C-N
1030	W	C-O, C-O-C, C-N
950	W	N-O, C-H
890	M	CH, N-H
820	M	CH, N-H
750	M	CH, C=C-H
690	W	CH, CH_2, CN

SAMPLE NO. 27-015

WAVE NO. CM1	INTENSITY	INFERENCE
2900	W	-C-C-, alkanes
2050	W	$-C\equiv C$

SAMPLE NO. 27-016

WAVE NO. CM1	INTENSITY	INFERENCE
2900	W	-C-C, Alkane
2350	W	P-H, $N^{+}H$

SAMPLE NO. 27-017

WAVE NO. CM^1	INTENSITY	INFERENCE
3010	M	-C=C-, -OH, NH
2900	W	-C-C, alkanes
2810	W	N-C-H, $-O-CH_3$
2710	W	$N-CH_3$, amines
2610	W	SH, Sulfur
2450	W	N^+H
2080	W	$C=N\pm H$
1370	W	CH, -OH
1300	W	CN,OH

SAMPLE NO. 27-018

WAVE NO. CM^1	INTENSITY	INFERENCE
3100	W	C_6H_6 Para, Meta, Ortho aromatics
2880	M	CH, OH...0, $O-CH_3$
2700	W	$N-CH_3$, Amines
2600	W	SH, Sulfur
2520	W	SH
2340	W	P-H, N ± H
1710	M	R-CO-O-N, R-CO-OSH, -CO-O, 0=C-C=O
1620	W	-COCH-OH, $C-O-CH-NH_2$, C=C
1400	W	$C-H(CO-CH_2)$, C-H(C=CH)
1380	W	CH, -OH
1270	M	CN, NO_2
770	M	CH, C=C-H
700	W	CH, CH_2, CN

SAMPLE NO. 27-019

WAVE NO. CM^1	INTENSITY	INFERENCE
2910	M	-C-C-
2310	W	P-H
1700	W	R-CO-ON, R-CO-OSH, -CO-O, O=C-C=O
1380	W	CH,-OH
1210	W	-C-O-C-, $-CH_3$

SAMPLE NO. 27-020

WAVE NO. CM^{1}	INTENSITY	INFERENCE
3310	BW	-CH
3080	W	C=C-H
2730	W	N-CH_3, Amines, OH...O
2610	W	SH, Sulfur
2350	W	P-H, N ± H
1780	W	C=O
1720	M	R-CO-ON, R-CO-OSH, -CO-O, O=C-C=O
1580	M	C=N; Aromatics, N ± H, C=C, N=O
1480	M	C=C; Aromatics
1380	M	-C-H, -OH
1200	M	-CH_3, C-O-C
1160	W	C-O, C-O-C, C-N
1070	W	C-O, C-O-C, C-N
880	W	CH, N-H
830	M	-CH, N-H
750	M	-CH, N-H
710	W	-CH, C=C-H
690	M	-CH_2, CH, CN

SAMPLE NO. 27-021

WAVE NO. CM^{1}	INTENSITY	INFERENCE
3050	M	$-CH=CH_2$, Napthalenes
2950	M	-C-C-, Alkane
2850	W	C-H, $O-CH_3$
2340	W	P-H, N ± H
1780	W	C=o
1720	M	R-CO-OH, N-CO-OSH, -CO-O, O=C-C=O
1610	W	-COCH-OH, $CO-CH-NH_2$, C=C
1400	M	$C-H(CO-CH_2)$, C-H(C=C-H)
1380	W	CH, -OH
1280	W	CN, NO_2
1170	W	C-O, C-O-C, C-N
1070	W	C-O, C-O-C, CN
1020	W	C-O, C-O-C, CN
950	W	N-O, C-H
880	M	CH, N-H
830	M	CH, N-H
750	M	CH, C≡C-H
680	W	CH, CH_2, CN

SAMPLE NO. 27-022

WAVE NO. CM^{1}	INTENSITY	INFERENCE
3100	BW	-OH, Moisture
2550	BW	SH, Moisture
2350	W	P-H, N ± H
2120	W	$C=N^{t}H$, C C
1700	S	R-CO-ON, R-CO-OSH, -CO-O, O=C-C=O
1580	W	C=N; Aromatic, N^{+}-H, C=C, N=O
1460	W	C=C, Aromatic
1400	W	$C-H(C-O-CH_3)$, C-H(C=C-H)
1320	W	C-N, NO, Aromatics
1250	M	-C-N, NO_2
1180	W	C-O, C-O-C, C-N
1090	W	C-O, C-O-C, C-N
1020	W	C-O, C-O-C, CN
840	W	CH, N-H
780	W	CH, C=C-H
740	W	CH, C=C-H
700	W	CH_2, CH, CN

SAMPLE NO. 27-023

WAVE NO. CM^1	INTENSITY	INFERENCE
3130	BW	-C=C-, OH, NH
1780	W	-C=C-C=O, -C=O
1700	S	R-CO-OH, R-CO-OSH, -CO-O, O=C-C=O
1580	M	C=N, Aromatics, N±H, C=C, N=O
1300	W	C-N, N-O Aromatics
1230	W	C-O-C, $-CH_3$
1180	W	C-O, C-O-C, CN
1100	W	C-O, C-O-C, CN
1020	W	C-O, -C-O-C, CN
830	W	CH, N-H
770	W	C-H, C=C-H, NH
740	W	CH, C=C-H
710	W	CH, CH_2, CH

SAMPLE NO. 27-024

WAVE NO. CM^{-1}	INTENSITY	INFERENCE
3250	BM	-OH; Acids
2810	M	N-C-H,-O-CH_3
2650	M	SH, Sulfur
2500	M	-OH...O, N^{+}-H
2350	W	P-H, $N^{t}H$
2120	W	C=N^{+}-H, C≡C
2000	W	-C≡C-; Alkyne
1920	W	C=O, N^{+}-H
1710	S	R-CO-ON, R-CO-OSH, -CO-O, O=C-C=O
1610	M	C=C, NH, C-O
1580	M	C=N; Aromatics, N^{+}-H, C=C, N=O
1500	M	C=C, N^{+}-H, N=O
1470	S	C=C
1400	S	-CH(CO-CH_2), CH(C=C-H)
1320	S	C-N, N-O; Aromatics
1250	S	C-N, NO_2
1180	S	C-O, C-O-C, C-N
1130	S	C-O, C-O-C, C-N
1100	M	C-O, C-O-C, C-N
1080	S	C-O, -C-O-C, CN
1030	S	C-O, -C-O-C, CN
1000	M	C-O, -C-O-C, CN
940	S	N-O, CH
800	S	N-H, CH, CH_2
750	S	CH, C=C-H
710	S	-CH_2
680	S	CH_2, CH, CN
660	S	-C-C, N-H

SAMPLE NO. 27-026

WAVE NO. CM^1	INTENSITY	INFERENCE
2950	W	-C-C; Alkanes
2850	W	-CH, O-CH$_3$
1670	W	N-C=O, Lactam, AR-CO-AR, Quinones

SAMPLE NO. 27-027

WAVE NO. CM^1	INTENSITY	INFERENCE
2950	W	-C-C-, Alkanes
2850	W	-CH, O-CH$_3$

SAMPLE NO. 27-032

WAVE NO. CM^1	INTENSITY	INFERENCE
3370	W	-OH
3300	W	C≡C-H
3250	W	-OH
3200	W	-OH
3120	W	C=C-H

SAMPLE NO. 27-034

WAVE NO. CM^{1}	INTENSITY	INFERENCE
3450	BM	-OH; Carboxylic Acids
3270	W	-OH
3070	S	$-CH=CH_2$, Aromatics
3010	S	-C=C-H, Aromatics, Alkenes
2930	S	-C-C-, Alkanes
2830	S	C-H, $O-CH_3$
2350	W	P-H, N^+-H
1950	W	C=O, N^+-H
1870	W	C=O, $C=N^+-H$
1740	S	R-CO-O-N, R-CO-O-SH, CO-O, O=C-C=O
1640	W	-COCHOH, $CO-CH-NH_2$, C=C
1580	M	C=N, Aromatics, N^+-H, C=C, N=O
1480	S	C=C, N^+-H, N=O
1440	S	C=C, Aromatics
1370	S	C-H, -OH
1200	S	-C-O-C-, $-CH_3$
1170	W	C-O, C-O-C, C-N
1140	W	C-O, C-O-C, C-N
1070	M	C-O, C-O-C, C-N
1010	M	CO, -C-O-C, CN
960	M	N-O, C-H
900	M	C=C-H, N-H
820	W	-CH, N-H
720	S	$-CH_2$
670	S	$-CH_2$, CH, CN

SAMPLE NO. 27-035

WAVE NO. CM^{1}	INTENSITY	INFERENCE
3300	BW	-OH
2940	S	-C-C- Alkanes
2840	S	-CH, O-CH$_3$
2230	W	-C≡C-, N$^+$-H
1820	W	C=O
1720	S	C=O
1580	W	C=N, Aromatics, N$^+$-H, C=C, N=O
1520	W	C=C, N^{t}H, N=O
1480	W	-C=C Aromatics
1440	S	-C=C Aromatics
1360	M	-C-H, -OH
1260	S	CN, NO$_2$
1170	M	C-O, C-O-C, C-N
1070	M	C-O, C-O-C, C-N
1020	M	C-O, C-O-C, C-N

APPENDIX II

IR SCREEN OF LC FRACTIONS

SAMPLE NO. 27-001 Fraction 1

WAVE NO. CM^1	INTENSITY	INFERENCE
2980	W	-C-C, Alkanes
2750	W	CH
1980	W	C=C, Aromatic Overtone
1800	W	C=C, Alkene, Aromatic Overtone
1740	W	C=C, Aromatic Overtone
1460	W	C=C, Aromatics
1220	W	$-CH_3$

SAMPLE NO. 27-001 Fraction 2

WAVE NO. CM^{1}	INTENSITY	INFERENCE
2320	W	C≡C
2250	W	C≡C, C-N=O
1880	W	Aromatic Overtone
1520	W	C=C, Aromatics
1500	W	C=C, Aromatics

SAMPLE NO. 27-001 Fraction 3

WAVE NO. CM^{1}	INTENSITY	INFERENCE
3030	M	C=C-H, Aromatics
2880	W	C-H
1880	W	Aromatic Overtone
1780	W	Aromatic Overtone
1700	W	Aromatic Overtone
1650	W	Aromatic Overtone
1580	W	C=C, Aromatics
1400	S	C=C-H, C-O-
1300	W	C-N Aromatic
1250	W	CH$_3$, C-N Aromatic
1180	W	C-F
1020	W	C-O Aromatic
930	W	C=C-H
880	W	C=C-H, C-H Aromatics, C-N
850	W	C=C=CH$_2$
820	W	C=C-H, C-H Aromatics
800	S	C=C-H, C-H Aromatics, N-H Aromatics, C-CL
750	W	C=C-H, C-H Aromatics, N-H Aromatics, C-CL
700	S	CH$_2$, C-CL

SAMPLE NO. 27-001 Fraction 4

WAVE NO. CM^1	INTENSITY	INFERENCE
3180	W	OH...O=C
2900	W	C-H
2830	W	C-H
1700	W	C=O, Aromatic Overtone, C=N
730	W	CH_2, NH, C=C-H; C-C

SAMPLE NO. 27-001 Fraction 5

WAVE NO. CM^{1}	INTENSITY	INFERENCE
3500	W	-OH, NH
3420	W	N-H
2230	W	C=N±H
2200	W	C≡C, C=N±H
1740	W	C=O, Aromatic Overtone
1700	W	C=O
1520	W	C=C Aromatic, C-N, NO_2
1450	W	CH_2-CO-, C=C-H, O-H, C-N, NO_2
1430	W	CH_2-CO-, C=C, O-H
1250	M	CH_3, C-O-C Aromatic
1150	W	CH_3, C-O, C-O-C, C-N
750	M	C=C-H, C-H Aromatic, NH Aromatics

SAMPLE NO. 27-001 Fraction 6

WAVE NO. CM^1	INTENSITY	INFERENCE
2900	M	C-H, OH
2830	W	C-H, -OH, $-O-CH_3$
1770	M	C=O
1710	S	C=O
1670	W	C=O, Aromatic Overtone
1590	S	C=C Aromatic, N-H, C=N, NO_2, N=O
1430	M	CH_2-CO, -OH
1280	W	-OH, C-N, NO_2, N-O, P-O
900	W	C=C-H Aromatics, CN, S-O
760	W	C=C-H Aromatic, N-H, S-O
730	W	CH_2
680	W	C-H, N-H, S-O

SAMPLE NO. 27-001 Fraction 7

WAVE NO. CM^{1}	INTENSITY	INFERENCE
3080	W	C-H Aromatics, -OH
2800	W	-OH, O-CH$_3$, CHO Overtone
2650	W	OH...O=C, -O-C-H
2550	W	OH...O=C, P-H
2350	W	P-H
1240	W	CH$_3$, -OH, C-O-C, C-N N-O, C-O
1220	W	CH$_3$, C-O-C, C-N Aromatics

SAMPLE NO. 27-001 Fraction 8

WAVE NO. CM^{1}	INTENSITY	INFERENCE
3600	W	-OH
3530	W	-OH, N-H
3420	W	N-H
2900	W	C-H, OH...O=C
2450	W	N±H
2300	W	C=N±H
1750	M	C=O
1450	W	$-CH_2-CO$, C=C Aromatic, -OH
1400	W	$-CH_2-CO$, C=C-H, -OH
1350	W	$-CH_3$, -OH
1320	W	$-CH_3$, -OH
1280	W	-OH, C-O-C, C-N Aromatics
1250	W	$-CH_3$, C-O-C, C-N Aromatics, NO_2, N-O
1220	W	$-CH_3$, C-O-C, C-N Aromatics, N-O
1200	W	$-CH_3$, C-O-C, C-N Aromatics, N-O
1120	W	C-O, C-O-C, CN

SAMPLE NO. 27-002 Fraction 1

WAVE NO. CM^{1}	INTENSITY	INFERENCE
3300	BS	$C\equiv C-H$, (Moisture)
2900	M	$C-H$
2850	M	$C-H$
2500	W	$OH\ldots O$
2400	W	$N\pm H$
1660	S	$C=C$, $C=O$
1480	W	$C=C$ Aromatics
1450	W	$C-H$
1420	W	$C-H$
1380	W	CH_3, $C-F$
1320	W	NO_2
1040	W	$C-O$, $C-O-C$

SAMPLE NO. 27-002 Fraction 2

WAVE NO. CM^{1}	INTENSITY	INFERENCE
2900	W	C-C, Alkanes
2850	W	C-H
1980	M	C=C, Aromatic Overtone
1900	M	Aromatic Overtone
1770	W	Aromatic Overtone
1750	W	Aromatic Overtone
1710	W	Aromatic Overtone
1580	W	C=C Aromatic
1520	W	C=C Aromatic
1480	W	C=C
1080	W	-CN Aromatic
1050	W	-CN-H

SAMPLE NO. 27-002 Fraction 3

WAVE NO. CM^1	INTENSITY	INFERENCE
3010	S	C=C-H Aromatics
2850	M	-C-H
2770	M	-C-H
2700	W	-C-H
1970	W	Aromatic Overtone
1940	W	Aromatic Overtone
1910	W	Aromatic Overtone
1810	W	Aromtic Overtone
1790	W	ARomatic Overtone
1650	M	C=C
1630	M	C=C
1600	S	N-H
1570	M	C=C Aromatic, N-H, NO$_2$, N=O
1550	M	C=C Aromatic
1540	M	C=C, NO$_2$ Aromatic
1490	M	C=C
1450	S	C-CH$_2$-CO
1420	S	C=C-H
1380	M	C-F
1310	M	C-N
1300	M	C-N
1180	S	C-O, C-O-C, CN
1120	W	C-O, C-O-C
1040	M	C-O-C
1010	M	C-O-C
950	M	C=C-H
880	M	C=C-H, C-H Aromatic, C-N
830	M	C=C-H, C-H ARomatic
800	S	C=C-H, C-H Aromatic, N-H Aromatic, C-CL
760	S	C=C-H, C-H Aromatic, N-H Aromatic, C-CL
740	S	C=C-H, C-H Aromatic, N-H Aromatic, C-CL
700	M	CH$_2$, C-CL
680	W	CH$_2$

SAMPLE NO. 27-002 Fraction 4

WAVE NO. CM^1	INTENSITY	INFERENCE
3400	W	N-H
3300	W	OH...OH
3050	W	C=C-H Aromatic
2900	W	CH_3, OH...O=C
2820	W	O-CH_3
1940	W	C=C=C, CN, Aromatic Overtone
1810	W	Aromatic Overtone
1530	W	C=C Aromatic, C=N
1460	M	NO_2, C=C
1410	M	C=C-H
1080	W	C-O, C-O-C
1040	W	C-O, C-O-C
1020	W	C-O, C-O-C
750	W	C=C-H, C-H Aromatic

SAMPLE NO. 27-002 Fraction 5

WAVE NO. CM^1	INTENSITY	INFERENCE
3400	BS	-OH
3080	W	C=C-H Aromatic
2900	M	CH_3, OH...O=C
2830	W	$O-CH_3$
2200	W	-N=C=O
1700	BS	C=O
1440	M	C=C
1340	W	-OH, CN, NO_2
1280	W	-OH, N-O
1150	W	CH_3, C-O, C-O-C, CN
1050	W	C-O, C-O-C
980	W	C=C-H
800	W	C=C-H, N-H, C-H Aromatic
760	W	C-H Aromatic
720	M	C=C-H, C-H Aromatic

SAMPLE NO. 27-002 Fraction 6

WAVE NO. CM^{1}	INTENSITY	INFERENCE
3300	BS	-OH
2900	S	NH, CH
2820	M	C-H, -OH, $-O-CH_3$
2200	W	C≡C
2050	W	C≡C, C=N±H
1980	W	Overtone
1740	S	C=O
1650	S	C=O
1540	S	C=O
1450	M	CH_2-CO, -OH
1150	W	CH_3, C-O, C-N, C-F
1280	S	-OH, CN, NO_2, N-O, P-O
1220	M	CH_3, C-O-C, C-N, N-O
1160	M	CH_3, C-O, C-O-C
1120	M	C-O, C-O-C, C-N
1040	W	C-O, C-O-C
820	M	C=C-H, C-H Aromatic
760	M	C=C-H, C-H ARomatic, N-H
720	M	CH_2
680	W	C-H, N-H, S-O

SAMPLE NO. 27-002 Fraction 7

WAVE NO. CM^{1}	INTENSITY	INFERENCE
3450	W	NH
3440	W	OH...OH, NH
3300	W	-OH
3180	W	OH...O=C
3100	W	C=C-H Aromatic
3010	W	C=C-H Aromatic
2900	M	NH, CH
2810	M	-OH, O-CH_3, CHO Overtone
1560	M	C=O

SAMPLE NO. 27-002 Fraction 8

WAVE NO. CM1	INTENSITY	INFERENCE
1730	M	Cannot be classified from spectrum
1300	W	
1260	W	
1220	W	
1080	W	
1020	W	
980	W	
940	W	
920	W	
900	W	
750	W	
610	W	

SAMPLE NO. 27-006 Fraction 1

WAVE NO. CM^{1}	INTENSITY	INFERENCE
3950	W	No Assignment
3410	S	NH
3310	M	$C\equiv C-H$
2500	W	OH...O
1990	W	Aromatic Overtones
1800	W	Aromatic Overtone
1720	W	Aromatic Overtone
1520	W	C=C Aromatics

SAMPLE NO. 27-006 Fraction 2

WAVE NO. CM^1	INTENSITY	INFERENCE
2930	S	C-C, Alkane
2880	M	C-H
1800	W	Aromatic Overtone
1720	W	Aromatic Overtone
1650	W	Aromatic Overtone
1360	M	C-F
1300	W	C-N
1270	W	C-N
1100	W	C-O, C-O-C
1030	W	C-O-C

SAMPLE NO. 27-006 Fraction 3

WAVE NO. CM^{1}	INTENSITY	INFERENCE
2460	W	OH...O=C
2350	M	C=N±H
1850	M	C=O, C-N
1540	M	C=C
1450	W	$C-CH_2-C-O$
1420	W	C=C-H
740	M	C=C-H, CH Aromatic, C-CL, N-H

SAMPLE NO. 27-006 Fraction 4

WAVE NO. CM^{1}	INTENSITY	INFERENCE
3400	BS	NH, Moisture
2900	S	CH_3, OH...O=C
2800	M	O-CH_3
2350	W	N$\pm$H
2250	W	N$\pm$H
1860	W	Aromatic Overtone
1660	W	Aromatic Overtone
1600	W	Aromatic Overtone
1450	M	NO_2, C=C
1250	W	CH_3, C-O-C, NH Aromatic
1200	W	CH_3, C-O, C-O-C
1120	W	C-O
1080	W	C-O, C-O-C
980	W	C=C-H

SAMPLE NO. 27-006 Fraction 5

WAVE NO. CM^{1}	INTENSITY	INFERENCE
2910	S	CH$_3$, OH...O=0C
2850	M	O-CH$_3$
1840	M	C=O
1710	M	C=O
1600	W	C=C
1260	M	CH$_3$, C-O-C, Aromatic
1080	M	C-O, C-O-C
1000	M	C-O
740	M	C=C-H, C-H Aromatic, NH Aromatic
700	W	C-CL
680	M	C-CL

SAMPLE NO. 27-006 Fraction 6

WAVE NO. CM^{1}	INTENSITY	INFERENCE
3510	S	-OH
3350	S	NH
3150	S	OH...O=C
3010	S	C-H
2930	S	N+H, CH
2800	S	CH
2600	M	SH
2300	M	N+H
1940	W	Aromatic Overtone
1740	W	C=O
1670	W	Aromatic Overtone
1630	W	Aromatic Overtone
1580	M	C=C Aromatics
1500	M	C=C, OH, CN
1450	M	CH_2-CO, -OH
1380	M	CH_3, -OH
1350	W	-OH, CN, NO_2
1320	W	-OH, CN, NO_2
1290	W	NO_2, N-O
1270	W	-OH, CN, NO_2, N-O, P-O
1250	S	CH_3, C-O-C, CN
1230	M	CH_3, C-O-C, CN, N-O
1200	S	CO-CH_3, C-O-C
1160	W	CH_3, C-O, C-O-C
1140	M	CH_3, C-O, C-O-C, CN
1090	M	C-O-, C-O-C, C-F
1050	S	C-O, C-O-C, C-N
990	M	C=C-H,
950	W	C=C-H, N-O
880	M	C=C-H, CH Aromatic
850	W	C=C-H, CH Aromatic
820	W	C=C-H, CH Aromatic
740	M	C=C-H, CH Aromatic, NH
680	S	C-CL

SAMPLE NO. 27-006 Fraction 7

WAVE NO. CM^{1}	INTENSITY	INFERENCE
3800	W	No Assignment
2900	W	OH...O=C
2730	W	N-CH, -OH
2630	W	OH
2580	W	N±H
2520	W	N±H
2300	M	-N=C=O
2150	W	C=N±H
2080	W	C=N±H
2020	W	-N=C=O
1980	W	No Assignment
1620	W	C=N
1580	W	NO_2, N=O
1180	W	C-O, C-O-C
1130	W	C-O, C-O-C
1030	W	C-O

SAMPLE NO. 27-006 Fraction 8

WAVE NO. CM^1	INTENSITY	INFERENCE
3450	BS	NH, Moisture
2960	W	C-H
2900	W	C-H
2850	W	$=OH...O=C$, $O=CH_3$
2730	W	N-C-H
2680	W	N±H
1800	W	Overtone
1750	W	Overtone
1680	W	Overtone
1640	W	Overtone
1620	W	Overtone
1000	W	C-O

SAMPLE NO. 27-024 Fraction 1

WAVE NO. CM1	INTENSITY	INFERENCE
2980	W	No Assignment
2900	S	C-H, Alkane
2800	M	C-H, Alkane

SAMPLE NO. 27-024 Fraction 2

WAVE NO. CM^1	INTENSITY	INFERENCE
3300	W	No Assignement
2900	M	C-C Alkane
2820	M	C-H
1740	W	Overtone, C=O
1610	W	Overtone
1530	W	C=C Aromatic
1450	W	$C-CH_2-CO$
1430	W	C=C-H
1360	W	CH_3
1280	W	C-O-C, C-N Aromatics

SAMPLE NO. 27-024 Fraction 3

WAVE NO. CM^1	INTENSITY	INFERENCE
2950	M	C-H
2540	M	OH...O=C
2480	W	N±H
2430	W	N±H
2310	M	N±H
1800	M	C=O
700	W	C=C-H

SAMPLE NO. 27-024 Fraction 4

WAVE NO. CM^1	INTENSITY	INFERENCE
2920	M	C-C
2840	M	C-H
2300	M	N±H
1750	M	C=O
1380	M	CH_3, -OH
1280	W	-OH
1180	W	CH_3
1100	W	C-O
1010	W	C-O-C, C-O

SAMPLE NO. 27-024 Fraction 5

WAVE NO. CM^1	INTENSITY	INFERENCE
2950	M	C-C
2750	W	C-H
2600	W	
2510	W	OH...O
2320	W	C≡C
2250	W	C≡C, C-N=O
1980	W	Overtone
1730	W	Overtone
1620	W	Overtone
1580	W	C=C, Aromatic
1500	W	C=C, Aromatic
1460	W	C=C
1410	W	C=C-H
1150	W	CH_3
1000	M	C-O-C
940	M	C=C-H
830	W	C=C-H, CH Aromatic
780	W	C=CH, CH Aromatic, NH Aromatic

SAMPLE NO. 27-024 Fraction 6

WAVE NO. CM^1	INTENSITY	INFERENCE	
3100	W	C=C-H	Alcohols
2550	M	C±H	Acids
2340	W		Esters
1990	W		
1900	W		
1850	W		
1800	W		
1700	S	C=O	
1640	M	C=O	
1620	W		
1610	W		
1580	W		
1510	W		
1470	M	-OH	
1440	S	$-CH_2-CO$	
1420	M	C=C-H	
1380	M	-OH	
1330	S	C-N, -OH	
1250	S	CH_3, C-O-C	
1180	S	CH_3, C-O, C-O-C	
1120	M	C-O, C-O-C	
1060	M	C-O, C-O-C	
1000	M	C=C-H, C-O	
920	S	C=C-H, NH	
800	S	C=C-H, CH, NH	
700	S	N-H	
680	W	C=C-H, N-H	
640	W	C-CL	

SAMPLE NO. 27-024 Fraction 7

WAVE NO. CM^1	INTENSITY	INFERENCE	
3300	Bs	NH, OH	Alcohols
2900	S	C-C	Acids
1710	S	C=O	Esters
1680	M	C=O	
1660	M	C=C	
1640	M	C=C, NH	
1620	M	C=C, NH	
1550	W	C=C	
1480	W	C=C	
1380	W	CH_3	
1240	S	CH_3	
1160	W	C-O, C-O-C	
1140	W	C-O, C-O-C	
1020	W	C-O, C-O-C	
750	M	C=C-H, CH	

SAMPLE NO. 27-024 Fraction 8

WAVE NO. CM^1	INTENSITY	INFERENCE
3120	W	
3030	W	C-H Aromatic
2920	W	C-H Aromatic
2900	S	C-C
2800	M	C-H
1920	W	Overtone
1890	W	Overotne
1850	W	Overtone
1820	W	Overtone
1770	W	Overtone
1740	W	Overtone
1680	W	C=N
1140	W	
850	W	
830	W	
780	W	

SAMPLE NO. 27-034 Fraction 1

WAVE NO. CM^1	INTENSITY	INFERENCE	
2900	S	C-C	Alkanes
2840	M	C-H	
1440	M	CH_3	
1370	M	CH_3	

SAMPLE NO. 27-034 Fraction 2

WAVE NO. CM^1	INTENSITY	INFERENCE
3000	W	
2940	W	
2910	M	C-C
2830	M	C-H
2550	W	

SAMPLE NO. 27-034 Fraction 3

WAVE NO. CM^1	INTENSITY	INFERENCE
3260	M	-OH
3220	S	
3100	S	C=C-H
3040	M	C-H
2090	W	
1840	W	
1590	M	C=C
1540	S	C=C Aromatic
1470	W	C=C
1460	W	
1420	W	
1410	W	
1360	M	-OH
1280	W	
1270	M	C-O-C
1250	M	CH_3
1160	M	C-O, C-O-C
1120	M	C-O, C-O-C
1050	W	
990	M	C=C-H
930	W	
910	W	
890	S	C=C-H, CH
780	S	C=C-H, CH

SAMPLE NO. 27-034 Fraction 4

WAVE NO. CM^1	INTENSITY	INFERENCE
3030	W	
3010	W	
2900	S	C-C
1440	M	CH_3
1020	M	C-O
950	M	C=C-H
900	M	C-H, C=C-H
750		

SAMPLE NO. 27-034 Fraction 5

WAVE NO. CM^{1}	INTENSITY	INFERENCE
3000	W	
2900	S	C-C
1800	W	
1720	S	C=O
1580	W	
1480	W	
1450	M	CH_3
1360	W	
1350	W	
1230	M	C-O-C

SAMPLE NO. 27-034 Fraction 6

WAVE NO. CM^1	INTENSITY	INFERENCE
3140	M	
2930	M	C-C
2820	M	C-H
1720	M	C=O
1680	M	Oventone
1600	M	Overtone
1570	M	C=C Aromatics
1530	M	C=C Aromatics
1470	M	CH$_3$
1380	W	
1060	S	C-O, C-O-C, CN
950	W	

SAMPLE NO. 27-034 Fraction 7

WAVE NO. CM1	INTENSITY	INFERENCE
3450	S	NH, OH
2900	S	C-C
2830	M	C-H
1730	M	C=O
2500	M	$-O-CH_3$, $N-CH_3$
1850	W	
1630	W	C=C
1370	W	-OH

SAMPLE NO. 27-034 Fraction 8

WAVE NO. CM^1	INTENSITY	INFERENCE
3250	W	
2920	M	C-C
1900	M	C=O
1850	M	C=O
1350	W	
1120	W	
1020	W	

SAMPLE NO. 27-035 Fraction 1

WAVE NO. CM^1	INTENSITY	INFERENCE
3200	W	
2900	S	C-C
2800	S	C-H
2300	W	
1440	M	C=C Aromatic
1340	M	CH_3
730	W	

SAMPLE NO. 27-035 Fraction 2

WAVE NO. CM^1	INTENSITY	INFERENCE
3150	W	
3000	W	
2910	S	C-C
2820	M	C-H
1880	W	Overtone
1780	W	Overtone
1680	W	Overtone
1600	W	Overtone
1550	W	C=C Aromatic
1530	W	C=C
1440	W	C=C
1380	W	
1340	W	
1150	W	
1030	W	

SAMPLE NO. 27-035 Fraction 3

WAVE NO. CM^1	INTENSITY	INFERENCE
2920	S	C-C
2830	M	C-H
2250	W	
2150	W	
170	W	
1630	W	C=C, Aromatic
1450	W	

SAMPLE NO. 27-035 Fraction 4

WAVE NO. CM^{1}	INTENSITY	INFERENCE
3110	W	
3000	W	
2900	S	C-C
2780	W	
1620	M	C=O
1440	M	C-H
750	M	C-H Aromatic
680	S	CH_3, C=C-H

SAMPLE NO. 27-035 Fraction 5

WAVE NO. CM^1	INTENSITY	INFERENCE
3400	S	NH
3220	W	
2910	S	C–C
2840	M	C–H
2750	W	
2650	W	
2580	W	
2520	W	
1880	M	C=O
1220	M	CH_3
1040	W	
1030	W	

SAMPLE NO. 27-035 Fraction 6

WAVE NO. CM^1	INTENSITY	INFERENCE
3300	BS	-OH
2950	S	C-C
2830	S	C-H
1750	S	C=O
1680	S	C=O
1640	M	C=C
1790	W	
1500	W	
1460	M	C-H, -OH
1420	M	C-H, -OH
1370	M	-OH
1270	S	CH_3
1180	W	
1150	M	C-O, C-O-C
1080	M	C-O, C-O-C
1040	M	C-O, C-O-C
1000	W	

SAMPLE NO. 27-035 Fraction 7

WAVE NO. CM^1	INTENSITY	INFERENCE
3300	BM	-OH
2930	S	C-C
2800	M	C-H
1750	W	Overtone
1470	W	-OH, C=C Aromatic
1400	W	CH$_3$
1250	W	CH$_3$
1080	BM	C-O, C-O-C

SAMPLE NO. 27-035 Fraction 8

WAVE NO. CM^1	INTENSITY	INFERENCE
2900	S	C-C
1750	M	C=O
1640	W	
1500	M	C=C
1450	W	-OH, C=C
1420	W	

COAL Fraction 1

WAVE NO. CM^{1}	INTENSITY	INFERENCE
2940	M	C-C
2850	M	C-H
1460	W	

COAL Fraction 2

WAVE NO. CM^{1}	INTENSITY	INFERENCE
2940	M	C-C
2850	W	C-H
2340	W	
1730	W	
1440	W	C=C
1260	W	
800	W	

COAL Fraction 3

WAVE NO. CM^1	INTENSITY	INFERENCE
2970	W	C-C
2930	W	C-C
2850	W	C-H
1460	W	CH_3
800	W	
730	W	

COAL Fraction 4

WAVE NO. CM^1	INTENSITY	INFERENCE
2900	W	C-C
1470	W	CH_3
800	W	
750	W	

COAL Fraction 5

WAVE NO. CM^1	INTENSITY	INFERENCE
2940	W	C-C
2830	W	C-H
2330	W	

COAL Fraction 6

WAVE NO. CM^1	INTENSITY	INFERENCE
2960	W	C-C
2900	W	C-C
2350	W	

COAL Fraction 7

WAVE NO. CM^1	INTENSITY	INFERENCE
3250	BW	-OH
2950	M	C-C
2850	M	C-H
2330	W	
1650	BW	C=O
1440	W	C=O

APPENDIX III

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